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The Landau-de Gennes theory of nematic liquid crystals: Uniaxiality versus Biaxiality

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The Landau-de Gennes theory of nematic liquid crystals: Uniaxiality versus Biaxiality

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Abstract

We study *small energy* solutions within the Landau-de Gennes theory for nematic liquid crystals, subject to Dirichlet boundary conditions. We consider two-dimensional and three-dimensional domains separately and study the correspondence between Landau-de Gennes theory and Ginzburg-Landau theory for superconductors. We treat uniaxial and biaxial cases separately. In the uniaxial case, topological defects correspond to the zero set and we obtain results for the location and dimensionality of the defect set, the solution profile near and away from the defect set. In the three-dimensional case, we establish the $C^{1,\alpha}$-convergence of uniaxial small energy solutions to a limiting harmonic map, away from the defect set, for some $0 < \alpha < 1$, in the *vanishing core limit*. Generalizations for biaxial small energy solutions are also discussed, which include physically relevant estimates for the solution and its scalar order parameters. This work is motivated by the study of defects in liquid crystalline systems and their applications.

1 Introduction

Nematic liquid crystals are examples of *mesophases* whose physical properties are intermediate between those of a typical liquid and a crystalline solid [10]. The constituent rod-like molecules have no translational order but exhibit a certain degree of long-range orientational ordering. Consequently, liquid crystals are anisotropic media and this makes them suitable for a wide range of physical applications and the subject of very interesting mathematical modelling [13].

The Landau-de Gennes theory is a general continuum theory for nematic liquid crystals [10, 28]. It describes the state of a nematic liquid crystal by a symmetric, traceless 3×3 matrix - the $\mathbf{Q}$-tensor order parameter, that is defined in terms of anisotropic macroscopic quantities, such as the magnetic susceptibility and the dielectric anisotropy. Nematic liquid crystals are said to be in the (a) *biaxial* phase when $\mathbf{Q}$ has three distinct eigenvalues, (b) *uniaxial* phase when $\mathbf{Q}$ has a pair of equal non-zero eigenvalues and (c) *isotropic* phase when $\mathbf{Q}$ has three equal eigenvalues or equivalently when $\mathbf{Q} = 0$. For a general biaxial phase, $\mathbf{Q}$ can be written in the form [15, 20]

$$\mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right) + r\left(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}\mathbf{I}\right) \quad s, r \in \mathbb{R};\ \mathbf{n},\mathbf{m}\in S^2, \tag{1}$$

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where s, r are scalar order parameters, $\mathbf{n}, \mathbf{m}$ are eigenvectors of $\mathbf{Q}$ and $\mathbf{I}$ is the 3×3 identity matrix. In the uniaxial phase, $\mathbf{Q}$ takes the simpler form of

$$\mathbf{Q} = s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\right) \quad s \in \mathbb{R};\ \mathbf{n} \in S^2 \tag{2}$$

where s is a scalar order parameter that measures the degree of orientational ordering about the distinguished eigenvector $\mathbf{n}$.

The Landau-de Gennes energy functional, $\mathcal{I}_{\mathcal{LG}}$, is a nonlinear integral functional of $\mathbf{Q}$ and its spatial derivatives. In the absence of any surface energies or external fields, $\mathcal{I}_{\mathcal{LG}}$ is given by [10, 20]

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}] = \int_\Omega \frac{1}{2}|\nabla \mathbf{Q}|^2 + \frac{f_B(\mathbf{Q})}{L_{el}}\ dV \tag{3}$$

where Ω is the domain, $f_B(\mathbf{Q})$ is the *bulk* energy density that dictates the preferred phase - isotropic, uniaxial or biaxial, L_{el} is a positive material-dependent elastic constant and $|\nabla \mathbf{Q}|^2$ is an *elastic* energy density that penalizes spatial inhomogeneities. The equilibrium, physically observable configurations correspond to either global or local Landau-de Gennes energy minimizers, subject to the imposed boundary conditions.

In this paper, we study sequences of *small energy* solutions $\left\{\mathbf{Q}^{L_{el}}\right\}$ in the limit $L_{el} \to 0$. Small energy solutions are classical solutions of the Euler-Lagrange equations associated with the energy functional (3) and they have small energy in the sense that

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}^{L_{el}}] \leq \mathcal{I}_{\mathcal{LG}}[\mathbf{Q}^0] \tag{4}$$

where $\mathbf{Q}^0$ is a limiting harmonic map [15]. Such small energy sequences include global energy minimizers. We emphasize on *uniaxial* small energy sequences in this paper because a rigorous study of uniaxial solutions is the first step in the mathematical analysis of arbitrary solutions and the interplay between biaxiality and uniaxiality. Secondly, uniaxial small energy solutions exist - this is known both analytically and numerically [19, 23, 25], examples of which include the well-known *radial hedgehog* solutions. Our results can be used to understand these solution structures and the nature of their singularities, making this a physically relevant and mathematically challenging problem. We also point out that there are two widely-used continuum theories for purely uniaxial liquid crystal phases - the *Oseen-Frank* theory and the *Ericksen* theory [13, 14, 8, 12] and uniaxiality is one of the most frequently used assumptions in the theoretical study of liquid crystalline systems, even in the context of applications. Our analysis does extend to the biaxial case although our results in the biaxial case are weaker due to technical difficulties.

The paper is organized as follows. In Section 2, we introduce some basic notation and terminology. In Section 3, we study Landau-de Gennes minimizers on two-dimensional (2D) domains and establish a $1-1$ correspondence between Landau-de Gennes theory and Ginzburg-Landau theory. In Section 4, we recall useful results from [15] in a three-dimensional (3D) framework that are crucial for the development of this paper. The results in [15] are for global Landau-de Gennes energy minimizers. We demonstrate that these results are also valid for small energy sequences (4) and this is a non-trivial observation, since results for global energy minimizers don't necessarily carry over to special sequences of solutions. In Section 5, we study uniaxial small energy solutions on 3D domains in the low-temperature regime. There are important differences between the $2D$ and $3D$ cases and the standard Ginzburg-Landau techniques do not extend to the $3D$ case. We derive the governing equations for uniaxial solutions and the governing equations reduce to the harmonic map equations in the limit of constant scalar order parameter. The scalar order parameter s vanishes at the defect locations (see (2) and the defect locations are prescribed in terms of the singular set of a *limiting harmonic map*. Using asymptotic methods, we show that the leading eigenvector $\mathbf{n}$ (see (2)) necessarily has a radial-hedgehog type of profile in the immediate neighbourhood of each isolated point defect. Our result is analogous to a powerful result on singularity profiles in [5], where the authors work within the Oseen-Frank theory for uniaxial liquid crystals with constant order parameter s. In Section 6, we study the qualitative properties of uniaxial small energy solutions away from the defect set, in the *vanishing core limit*. This limit is expressed in terms of a dimensionaless parameter $L = \frac{L_{el}}{a_{NI}^2 R^2}$, where R is a measure of the domain size and a_{NI}^2 is a characteristic constant related to the nematic-isotropic transition temperature [22, 19]. The limit $L \to 0$ is particularly relevant for macroscopic domains that are much larger than typical defect core sizes. We adapt the small energy regularity theorem of [7] to the Landau-de Gennes framework and prove the $C^{1,\alpha}$-convergence of small energy uniaxial solutions to a limiting harmonic map, away from the defect set, as $L \to 0$. This convergence result encodes quantitative information about the corresponding scalar order parameter. In Section 7, we discuss various generalizations of our results to the completely general biaxial case. The uniaxial case in $3D$ can be viewed as a generalized Ginzburg-Landau theory from $\mathbb{R}^3$ to $\mathbb{R}^3$ although there are important technical differences. However, the biaxial case presents a whole host of new mathematical difficulties; there are five degrees of freedom in the biaxial case and the additional degrees of freedom give us more possibilities, particularly in the context of defects. Finally, in Section 8, we discuss certain directions for future research. The methods in this paper contribute to the development of a generalized Ginzburg-Landau theory from $\mathbb{R}^3$ to higher dimensions ($\mathbb{R}^5$ in this case), for non-standard non-convex multi-well bulk potentials.

2 Preliminaries

Let $\bar{S}_d \subset \mathbb{M}^{d\times d}$ denote the space of symmetric, traceless $d \times d$ matrices i.e.

$$\bar{S}_d \stackrel{def}{=} \left\{ \mathbf{Q} \in \mathbb{M}^{d\times d}; \mathbf{Q}_{ij} = \mathbf{Q}_{ji},\ \mathbf{Q}_{ii} = 0 \right\}$$

where we have used the Einstein summation convention; the Einstein convention will be used in the rest of the paper. The corresponding matrix norm is defined to be

$$|\mathbf{Q}| \stackrel{def}{=} \sqrt{\mathrm{tr}\mathbf{Q}^2} = \sqrt{\mathbf{Q}_{ij}\mathbf{Q}_{ij}} \quad i,j = 1\ldots d.$$

We take our domain Ω to be either a two-dimensional or three-dimensional i.e. $d = 2$ or $d = 3$, bounded, connected and simply-connected set with smooth boundary, $\partial\Omega$. We work with the simplest form of the bulk energy density, f_B, in (3) that allows for a first-order nematic-isotropic phase transition [20]. We focus on the low-temperature regime; the function f_B is bounded from below and can be written as

$$f_B(\mathbf{Q}) = -\frac{a^2}{2}\mathrm{tr}\left(\mathbf{Q}^2\right) - \frac{b^2}{3}\mathrm{tr}\left(\mathbf{Q}^3\right) + \frac{c^2}{4}\left(\mathrm{tr}(\mathbf{Q}^2)\right)^2 + C(a^2, b^2, c^2) \tag{5}$$

where $a^2, b^2, c^2 \in \mathbb{R}^+$ are material-dependent and temperature-dependent positive constants and $C(a^2, b^2, c^2)$ is a positive constant that ensures $f_B(\mathbf{Q}) \geq 0$ for all $\mathbf{Q}$-tensors. We note that $C(a^2, b^2, c^2)$ plays no role in energy minimization, in either spatially homogeneous or inhomogeneous cases and the negative coefficient of $\mathrm{tr}\left(\mathbf{Q}^2\right)$ incorporates the fact that we are working below the nematic-isotropic transition temperature. In $2D$, f_B attains its minimum on the set of $\mathbf{Q}$-tensors defined by

$$\mathbf{Q}_2 = \left\{ \mathbf{Q} \in \bar{S}_2; \mathbf{Q} = \sqrt{\frac{2a^2}{c^2}} \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{2}\mathbf{I}_2 \right) \right\} \tag{6}$$

where $\mathbf{n} \in S^1$ and $\mathbf{I}_2$ is the 2×2 identity matrix. In $3D$, f_B attains its minimum on the set of uniaxial $\mathbf{Q}$-tensors given by [16]

$$\mathbf{Q}_{min} = \left\{ \mathbf{Q} \in \bar{S}_3, \mathbf{Q} = s_+ \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I} \right) \right\} \tag{7}$$

with $\mathbf{n} \in S^2$, $\mathbf{I}$ is the 3×3 identity matrix and

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \tag{8}$$

We work with *strong anchoring conditions* or Dirichlet boundary conditions. The prescribed boundary condition $\mathbf{Q}_b$ is given by

$$\mathbf{Q}_b = s_{eq}(d) \left(\mathbf{n}_b \otimes \mathbf{n}_b - \frac{1}{d}\mathbf{I} \right) \tag{9}$$

where d is the domain dimension, $\mathbf{I}$ is the corresponding identity matrix,

$$s_{eq}(d) = \begin{cases} \sqrt{\frac{2a^2}{c^2}}, & d = 2 \\ s_+, & d = 3, \end{cases} \tag{10}$$

$\mathbf{n}_b \in W^{1,2}(\Omega; M)$ ($M = S^1$ in $2D$ and $M = S^2$ in $3D$) is a unit-vector field with non-zero topological degree, when viewed as a map from $\partial\Omega$ to M. Clearly, $\mathbf{Q}_b \in \mathbf{Q}_{\min}$ in $3D$, where $\mathbf{Q}_{\min}$ has been defined in (7). We define our admissible space to be

$$\mathcal{A}_{\mathbf{Q}} = \left\{ \mathbf{Q} \in W^{1,2}\left(\Omega; \bar{S}_d\right); \mathbf{Q} = \mathbf{Q}_b \text{ on } \partial\Omega, \ \text{ with } \mathbf{Q}_b \text{ as in (9)} \right\}, \tag{11}$$

where $W^{1,2}\left(\Omega; \bar{S}_d\right)$ is the Sobolev space of square-integrable $\mathbf{Q}$-tensors in d-dimensions ($d = 2$ or $d = 3$ in this paper) with square-integrable first derivatives [9]. The existence of global energy minimizers for $\mathcal{I}_{\mathcal{LG}}$ in the admissible space $\mathcal{A}_{\mathbf{Q}}$ follows readily from the direct methods in the calculus of variations [16, 15]. For completeness, we recall that the $W^{1,2}$-norm is given by $\|\mathbf{Q}\|_{W^{1,2}(\Omega)} = \left(\int_\Omega |\mathbf{Q}|^2 + |\nabla \mathbf{Q}|^2 \, dx \right)^{1/2}$. In addition to the $W^{1,2}$-norm, we also use the L^∞-norm in this paper, defined to be $\|\mathbf{Q}\|_{L^\infty(\Omega)} = \text{ess sup}_{\mathbf{x} \in \Omega} |\mathbf{Q}(\mathbf{x})|$.

Finally, we introduce the concept of a *"limiting uniaxial harmonic map"* in $3D$, $\mathbf{Q}^0 : \Omega \to \mathbf{Q}_{min}$; $\mathbf{Q}^0$ is defined to be

$$\mathbf{Q}^0 = s_+ \left(\mathbf{n}_0 \otimes \mathbf{n}_0 - \frac{1}{3}\mathbf{I} \right) \tag{12}$$

where $\mathbf{n}_0$ is a minimizer of the Dirichlet energy

$$I_{OF}[\mathbf{n}] = \int_\Omega |\nabla \mathbf{n}|^2 \, dV \tag{13}$$

on $\Omega \subset \mathbb{R}^3$, in the admissible space

$$\mathcal{A}_{\mathbf{n}} = \left\{ \mathbf{n} \in W^{1,2}\left(\Omega; S^2\right); \ \mathbf{n} = \mathbf{n}_b \ on \ \partial\Omega \right\}. \tag{14}$$

The terminology *limiting harmonic map* stems from the fact that $\mathbf{n}_0$ is a harmonic unit-vector field [24] and it can be shown that $\mathbf{Q}^0$ is a global minimizer of $\mathcal{I}_{\mathcal{LG}}$ in the restricted class $\mathcal{A}_{\mathbf{Q}} \cap \{\mathbf{Q}_{\min}\}$ [5],[13]. We use the limiting harmonic map $\mathbf{Q}^0$ to study the inter-relationship between the Landau-de Gennes theory and the Oseen-Frank theory for nematic liquid crystals. The Oseen-Frank theory is the simplest continuum theory for nematic liquid crystals, restricted to uniaxial phases with constant scalar order parameter [10]. Working within the one-constant approximation, the Oseen-Frank energy reduces to the Dirichlet energy in (13) and $\mathbf{n}_0$, and hence $\mathbf{Q}^0$, is a global Oseen-Frank energy minimizer in the admissible space $\mathcal{A}_{\mathbf{n}}$.

3 The $2D$ case

Let $\Omega \subset \mathbb{R}^2$ be a bounded, connected and simply-connected domain with smooth boundary. Then $\mathbf{Q} \in \bar{S}_2$ can be written as

$$\mathbf{Q} = \lambda \left(\mathbf{n} \otimes \mathbf{n} - \mathbf{m} \otimes \mathbf{m} \right) \tag{15}$$

where $\lambda \in \mathbb{R}$ and $\mathbf{n}, \mathbf{m}$ are the two orthonormal eigenvectors of $\mathbf{Q}$. We note that there are only two degrees of freedom in the representation (15) and hence we can think of $\mathbf{Q}$ as being a map $\mathbf{Q} : \Omega \to \mathbb{R}^2$. Using the identity, $\delta_{ij} = \mathbf{n}_i \mathbf{n}_j + \mathbf{m}_i \mathbf{m}_j$, we can re-write (15) as

$$\mathbf{Q} = 2\lambda \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{2}\mathbf{I}_2 \right) \tag{16}$$

where $\mathbf{I}_2$ is the 2×2 identity matrix. We can also think of $\mathbf{Q} \in \bar{S}_2$ as being a symmetric, traceless 3×3 matrix: $\mathbf{Q} = (\lambda + \frac{1}{6})\mathbf{n} \otimes \mathbf{n} + (\frac{1}{6} - \lambda)\mathbf{m} \otimes \mathbf{m} - \frac{1}{3}\mathbf{z} \otimes \mathbf{z} \in \bar{S}$ where $\mathbf{z}$ is the unit-vector in the z-direction.

Straightforward calculations show that

$$\begin{aligned} &|\mathbf{Q}|^2 = 2\lambda^2 \\ &\mathrm{tr}\mathbf{Q}^3 = \mathbf{Q}_{ij}\mathbf{Q}_{jp}\mathbf{Q}_{pi} = 0 \quad i,j,p = 1,2. \end{aligned} \tag{17}$$

Then the Landau-de Gennes energy functional in (3) simplifies to

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}] = \int_\Omega \frac{1}{2}|\nabla \mathbf{Q}|^2 + \frac{1}{L_{el}} \left\{ -\frac{a^2}{2}\mathrm{tr}\mathbf{Q}^2 + \frac{c^2}{4}(\mathrm{tr}\mathbf{Q}^2)^2 \right\} \, dV \tag{18}$$

for two-dimensional domains. The corresponding Euler-Lagrange equations are -

$$\mathbf{Q}_{ij,kk} = \frac{1}{L_{el}} \left(-a^2 + c^2 |\mathbf{Q}|^2 \right) \mathbf{Q}_{ij} \quad i,j = 1,2 \tag{19}$$

and using the scaling $\widetilde{\mathbf{Q}} = \sqrt{\frac{c^2}{a^2}}\mathbf{Q}$, we obtain the following system of partial differential equations -

$$\begin{aligned} &\widetilde{\mathbf{Q}}_{ij,kk} = \frac{a^2}{L_{el}} \left(\left| \widetilde{\mathbf{Q}} \right|^2 - 1 \right) \widetilde{\mathbf{Q}}_{ij} \quad i,j,k = 1,2 \\ &\widetilde{\mathbf{Q}} = \sqrt{2} \left(\mathbf{n}_b \otimes \mathbf{n}_b - \frac{1}{2}\mathbf{I} \right) \; on \; \partial\Omega. \end{aligned} \tag{20}$$

This is equivalent to the Ginzburg-Landau equations for superconductors in two dimensions [26] and we are interested in the asymptotic properties of global energy minimizers either in the limit $a^2 \to \infty$ (low temperature regime) or $L_{el} \to 0^+$.

Let $\mathbf{Q}^{L_{el}}$ be a global minimizer of $\mathcal{I}_{\mathcal{LG}}$ in (18), in the admissible space $\mathcal{A}_{\mathbf{Q}} = \left\{ \mathbf{Q} \in W^{1,2}\left(\Omega; \bar{S}_2\right); \mathbf{Q} = s_{eq}\left(\mathbf{n}_b \otimes \mathbf{n}_b - \frac{1}{2}\mathbf{I}\right) \ on\ \partial\Omega \right\}$ for a fixed $L_{el} > 0$, where s_{eq} has been defined in (10). Then $\mathbf{Q}^{L_{el}}$ is necessarily of the form

$$\mathbf{Q}^{L_{el}}(\mathbf{x}) = s^{L_{el}}(\mathbf{x})\left(\mathbf{n}^{L_{el}}(\mathbf{x}) \otimes \mathbf{n}^{L_{el}}(\mathbf{x}) - \frac{1}{2}\mathbf{I}_2\right) \tag{21}$$

for some scalar function $s^{L_{el}} : \bar{\Omega} \to \mathbb{R}$, $\mathbf{n}^{L_{el}} \in W^{1,2}\left(\Omega; S^1\right)$ and $\mathbf{Q}^{L_{el}}$ is a classical solution of (20). Let $\Theta_{L_{el}} = \left\{\mathbf{x} \in \Omega; s^{L_{el}}(\mathbf{x}) = 0\right\}$ denote the isotropic set of $\mathbf{Q}^{L_{el}}$. We have a topologically non-trivial boundary condition in (20), since $\mathbf{n}_b$ has non-zero topological degree when viewed as a map from $\partial\Omega$ to S^1. Hence, the unit-vector field $\mathbf{n}^{L_{el}}$ necessarily has interior discontinuities and let $S_{\mathbf{n}}$ denote the defect set of $\mathbf{n}^{L_{el}}$. Then

$$S_{\mathbf{n}} \subset \Theta_{L_{el}} \tag{22}$$

since $\mathbf{Q}^{L_{el}}$ is well-defined at all points inside $S_{\mathbf{n}}$. In what follows, we use existing results in the mathematical literature for Ginzburg-Landau theory in two dimensions, to make predictions about the structure and location of the isotropic set and the far-field properties of global energy minimizers.

Dimension of $\Theta_{L_{el}}$ [2, 6]: The isotropic set $\Theta_{L_{el}}$ consists of $|D|$ isolated points, $\left\{a_1, \dots a_{|D|}\right\}$, where D is the topological degree of the boundary condition $\mathbf{Q}_b$ in (9).

The configuration $\left(a_1, \dots a_{|D|}\right)$ minimizes the renormalized energy W over $(b_1, \dots b_{|D|}) \in \Omega^{|D|}$, which is defined by

$$W(b_1, \dots b_{|D|}) = -2\pi \sum_{i \neq j} \log|b_i - b_j| - 2\pi \sum_{i,j} R(b_i, b_j) \tag{23}$$

where $R(\mathbf{x}, \mathbf{y}) = \Psi(\mathbf{x}, \mathbf{y}) - \log|\mathbf{x} - \mathbf{y}|, \mathbf{x}, \mathbf{y} \in \mathbb{R}^2$ and $\Psi(\mathbf{x}, \mathbf{y})$ is given by the solution of an explicit boundary-value problem [3, 26].

Far-field behaviour [3, 26]: Let $\left\{\mathbf{Q}^{L_{el}^k}\right\}$ denote a sequence of global energy minimizers for (18), where $L_{el}^k \to 0^+$ as $k \to \infty$. Then (up to a subsequence),

$$\mathbf{Q}^{L_{el}^k} \to \mathbf{Q}^* \ in\ C^{1,\alpha}\left(\bar{\Omega} \setminus \Theta_{L_{el}}\right), \quad \forall \alpha < 1 \ and\ in\ W^{1,p}(\Omega),\ \forall p \in [1, 2)$$

for some $\mathbf{Q}^* \in \cap_{1 \leq p < 2} W^{1,p}\left(\Omega; S^1\right)$. The limit $\mathbf{Q}^*$ is the canonical harmonic map associated with $a_1, \dots a_{|D|}$ and the degrees $\operatorname{sgn} D, \dots \operatorname{sgn} D$.

The interested reader is referred to [3, 26] for the proofs.

4 Preliminaries for $3D$ case

Let $\Omega \subset \mathbb{R}^3$ be a bounded, connected and simply-connected domain with smooth boundary. An arbitrary $\mathbf{Q}$-tensor field, $\mathbf{Q} : \Omega \to \bar{S}_3$ can be written as

$$\mathbf{Q} = \sum_{i=1}^{3} \lambda_i \mathbf{e}_i \otimes \mathbf{e}_i \quad \sum_i \lambda_i = 0$$

where $\mathbf{e}_i$ are the orthonormal eigenvectors, λ_i are the corresponding eigenvalues and in contrast to the $2D$ case, $\mathrm{tr}\mathbf{Q}^3 \neq 0$ in general.

We consider the Landau-de Gennes energy functional, $\mathcal{I}_{\mathcal{LG}}$ in (3), in the admissible space $\mathcal{A}_{\mathbf{Q}} = \left\{\mathbf{Q} \in W^{1,2}\left(\Omega; \bar{S}_3\right); \mathbf{Q} = \mathbf{Q}_b \textit{ on } \partial\Omega\right\}$. The corresponding Euler-Lagrange equations are

$$L_{el}\Delta\mathbf{Q}_{ij} = -a^2\mathbf{Q}_{ij} - b^2\left(\mathbf{Q}_{ik}\mathbf{Q}_{kj} - \frac{\delta_{ij}}{3}\mathrm{tr}(\mathbf{Q}^2)\right) + c^2\mathbf{Q}_{ij}\mathrm{tr}(\mathbf{Q}^2) \quad i,j = 1,2,3, \tag{24}$$

where the term $b^2\frac{\delta_{ij}}{3}\mathrm{tr}(\mathbf{Q}^2)$ is a Lagrange multiplier associated with the tracelessness constraint. It follows from standard arguments in elliptic regularity that all solutions are actually classical solutions of (24) and they are smooth and real analytic on Ω, up to the boundary [15].

The equations (24) can be non-dimensionalized as follows. Define $R = \min_{\mathbf{x},\mathbf{y}\in\partial\Omega}|\mathbf{x}-\mathbf{y}|$ and introduce the following scaled variables:

$$\bar{\mathbf{r}} = \frac{\mathbf{r}}{R};$$
$$\bar{a}^2 = \frac{a^2}{a_{NI}^2},\ \bar{b}^2 = \frac{b^2}{a_{NI}^2},\ \bar{c}^2 = \frac{c^2}{a_{NI}^2} \tag{25}$$

where $a_{NI}^2 = \frac{b^4}{27c^2}$. In terms of these re-scaled variables, the equations (24) reduce to

$$\frac{L_{el}}{a_{NI}^2R^2}\frac{\partial^2\mathbf{Q}_{ij}}{\partial\bar{\mathbf{r}}_k\partial\bar{\mathbf{r}}_k} = -\bar{a}^2\mathbf{Q}_{ij} - \bar{b}^2\left(\mathbf{Q}_{ik}\mathbf{Q}_{kj} - \frac{\delta_{ij}}{3}\mathrm{tr}(\mathbf{Q}^2)\right) + \bar{c}^2\mathbf{Q}_{ij}\mathrm{tr}(\mathbf{Q}^2) \quad i,j = 1,2,3. \tag{26}$$

We define the dimensionless parameter

$$L = \frac{L_{el}}{a_{NI}^2R^2} \tag{27}$$

where $\xi_u = \sqrt{\frac{L_{el}}{a_{NI}^2}}$ is a uniaxial correlation length related to defect core size [19]. We note that the system (26) has an associated dimensionless free energy:

$$\overline{\mathcal{I}_{\mathcal{LG}}}[\mathbf{Q}] = \int_{\bar{\Omega}} \frac{1}{2}|\nabla\mathbf{Q}|^2 + \frac{\overline{f_B}(\mathbf{Q})}{L}\, d\bar{V} \tag{28}$$

where L is defined in (27), $\overline{\mathcal{I}_{\mathcal{LG}}} = \frac{\mathcal{I}_{\mathcal{LG}}}{a_{NI}^2R^3}$, $\overline{f_B} = \frac{f_B}{a_{NI}^2}$ and f_B has been defined in (5), $\bar{\Omega}$ and $d\bar{V}$ are the re-scaled domain and volume element respectively. The re-scaled bulk energy density $\overline{f_B}$ attains its minimum on the set $\mathbf{Q}_{\min}$ as before

$$\mathbf{Q}_{min} = \left\{\mathbf{Q} \in \bar{S}_3, \mathbf{Q} = s_+\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right)\right\} \tag{29}$$

where s_+ has been defined in (8). In what follows, we drop the bars from the re-scaled variables for convenience and all subsequent results should be interpreted in terms of the dimensionless quantities above.

We briefly comment on limiting harmonic maps in a $3D$ setting: $\mathbf{Q}^0 = s_+\left(\mathbf{n}_0\otimes\mathbf{n}_0 - \frac{1}{3}\mathbf{I}\right)$ where $\mathbf{n}_0$ is an energy minimizing harmonic map in the admissible space $\mathcal{A}_{\mathbf{n}} = \left\{\mathbf{n} \in W^{1,2}(\Omega; S^2); \mathbf{n} = \mathbf{n}_b \textit{ on } \partial\Omega\right\}$. We note that $\mathbf{Q}^0 \in \mathcal{A}_{\mathbf{Q}}$, where the admissible space $\mathcal{A}_{\mathbf{Q}}$ has been defined in (11). Let S_0 denote the singular set of $\mathbf{n}_0$ (and hence, of $\mathbf{Q}^0$). Then S_0 consists of precisely $|D|$ isolated point singularities [5, 24], where D is the topological degree of $\mathbf{n}_b$.

Let $\mathbf{Q}^{L_k}$ be a sequence of solutions for the re-scaled system (26), where $L_k \to 0^+$ as $k \to \infty$. Then we refer to $\left\{\mathbf{Q}^{L_k}\right\}$ as a small energy sequence if

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}^{L_k}] \leq \mathcal{I}_{\mathcal{LG}}[\mathbf{Q}^0] \quad \forall L_k > 0. \tag{30}$$

The limit $L \to 0^+$ is referred to as the *vanishing core limit* in the rest of the paper since it is relevant for macroscopic domains with $R >> \xi_u$ [22]. We, next, quote important results from [15, 16] that are crucial for the analysis of small energy solutions, away from S_0, in the vanishing core limit.

Maximum principle [16]: Let $\mathbf{Q}$ be an arbitrary solution of the Euler-Lagrange equations (26) in the space $\mathcal{A}_{\mathbf{Q}}$. Then

$$\|\mathbf{Q}\|_{L^\infty(\Omega)} \leq \sqrt{\frac{2}{3}} s_+ \tag{31}$$

where s_+ has been defined in (29).

Strong convergence to $\mathbf{Q}^0$: Let $\Omega \subset \mathbb{R}^3$ be a bounded, connected and simply-connected domain with smooth boundary. Let $\left\{\mathbf{Q}^{L_k}\right\}$ be a small energy sequence in the admissible space $\mathcal{A}_{\mathbf{Q}}$ ($\mathcal{A}_{\mathbf{Q}}$ have been defined in (11)) where $L_k \to 0$ as $k \to \infty$. Then $\mathbf{Q}^{L_k} \to \mathbf{Q}^0$ strongly in $W^{1,2}\left(\Omega; \bar{S}_3\right)$ (upto a subsequence), where $\mathbf{Q}^0$ has been defined in (12).

Proof: This was demonstrated in [15] for sequences of global Landau-de Gennes energy minimizers $\left\{\mathbf{Q}^{L_k}\right\}$, where $L_k \to 0$ as $k \to \infty$. The same arguments also apply to small energy sequences (4).

Let $\left\{\mathbf{Q}^{L_k}\right\}$ be a small energy sequence in the admissible space $\mathcal{A}_{\mathbf{Q}}$. We recall that the limiting harmonic map $\mathbf{Q}^0 \in \mathcal{A}_{\mathbf{Q}}$. From the inequality (4) and the energy definition (3), we have that

$$\int_\Omega \frac{1}{2}|\nabla \mathbf{Q}^{L_k}|^2 \, dV \leq \int_\Omega \frac{1}{2}|\nabla \mathbf{Q}^{L_k}|^2 + \frac{f_B(\mathbf{Q}^{L_k})}{L_k} \, dV \leq \int_\Omega \frac{1}{2}|\nabla \mathbf{Q}^0|^2 \, dV = C(\Omega) s_+^2 \tag{32}$$

since $f_B(\mathbf{Q}^0) = 0$. The sequence of inequalities (32) shows that the $W^{1,2}$-norms of the $\mathbf{Q}^{L_k}$'s are bounded uniformly in L. Hence, we can extract a weakly convergent subsequence (also denoted by $\left\{\mathbf{Q}^{L_k}\right\}$) such that $\mathbf{Q}^{L_k}$ converges weakly to $\mathbf{Q}^1$ in $W^{1,2}$, for some $\mathbf{Q}^1 \in \mathcal{A}_{\mathbf{Q}}$ as $L_k \to 0$. Using the lower semicontinuity of the $W^{1,2}$-norm with respect to the weak convergence, we have that

$$\int_\Omega |\nabla \mathbf{Q}^1|^2 \, dV \leq \int_\Omega |\nabla \mathbf{Q}^0|^2 \, dV. \tag{33}$$

On the other hand, as $L_k \to 0$, we have $f_B(\mathbf{Q}^{L_k}(\mathbf{x})) \to 0$ for almost all $\mathbf{x} \in \Omega$ (see (32)). Therefore, the weak limit $\mathbf{Q}^1 \in \mathbf{Q}_{\min}$ and is of the form

$$\mathbf{Q}^1(\mathbf{x}) = s_+ \left(\mathbf{n}^1 \otimes \mathbf{n}^1 - \frac{1}{3}\mathbf{I}\right), \quad \mathbf{n}^1 \in S^2, a.e. \mathbf{x} \in \Omega \tag{34}$$

where s_+ has been defined in (8). We note that $|\nabla \mathbf{Q}^1|^2 = 2s_+^2 |\nabla \mathbf{n}^1|^2$ and $|\nabla \mathbf{Q}^0|^2 = 2s_+^2 |\nabla \mathbf{n}^0|^2$ and recall that $\mathbf{Q}^0$ is a global Landau-de Gennes energy minimizer in the restricted space $\mathcal{A}_{\mathbf{Q}} \cap \mathbf{Q}_{\min}$ to deduce that $\int_\Omega |\nabla \mathbf{Q}^1|^2 \, dV = \int_\Omega |\mathbf{Q}^0|^2 \, dV$ and hence,

$$\int_\Omega |\nabla \mathbf{Q}^0|^2 \, dV \leq \liminf_{L_k \to 0} \int_\Omega |\nabla \mathbf{Q}^{L_k}|^2 \, dV \leq \limsup_{L_k \to 0} \int_\Omega |\nabla \mathbf{Q}^{L_k}|^2 \, dV \leq \int_\Omega |\nabla \mathbf{Q}^0|^2 \, dV \tag{35}$$

from which the strong convergence result, $\mathbf{Q}^{L_k} \to \mathbf{Q}^0$ in $W^{1,2}$ follows. □

Interior and boundary monotonicity lemmas [15]: Let $\mathbf{Q}$ be an arbitrary solution of the Euler-Lagrange equations (26). Define the normalized energy on balls $B(\mathbf{x}, r) \subset \Omega = \{\mathbf{y} \in \Omega : |\mathbf{x} - \mathbf{y}| \leq r\}$:

$$\mathcal{F}(\mathbf{Q}, \mathbf{x}, r) = \frac{1}{r} \int_{B(\mathbf{x},r)} \frac{1}{2}|\nabla \mathbf{Q}|^2 + \frac{f_B(\mathbf{Q})}{L} \, dV.$$

Then we have the following interior monotonicity lemma:

$$\mathcal{F}(\mathbf{Q}, \mathbf{x}, r) \leq \mathcal{F}(\mathbf{Q}, \mathbf{x}, R) \quad \forall \mathbf{x} \in \Omega; \; r \leq R \; and \; B(\mathbf{x}, R) \subset \Omega. \tag{36}$$

Similarly, for $\mathbf{x}_0 \in \partial\Omega$, we define the region $\Omega_r = \bar{\Omega} \cap B(\mathbf{x}_0, r)$ with $r > 0$, and the corresponding normalized energy to be

$$\mathcal{E}(\mathbf{Q}, \mathbf{x}_0, r) = \frac{1}{r} \int_{\Omega_r} \frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{f_B(\mathbf{Q})}{L} \, dV.$$

Then there exists $r_0 > 0$ so that

$$\frac{d}{dr} \mathcal{E} \geq -C \left(a^2, b^2, c^2, \mathbf{Q}_b, r_0, \Omega \right) \quad 0 < r < r_0 \tag{37}$$

where the positive constant C is independent of L.

The proofs of (36) and (37) follow a standard pattern using the Pohozaev identity; complete details can be found in [15]. An immediate consequence of the strong convergence and the monotonicity lemmas is the following:

Convergence of bulk energy density away from S_0 [15]: Let $\left\{ \mathbf{Q}^{L_k} \right\}$ be a small energy sequence in the admissible space $\mathcal{A}_{\mathbf{Q}}$, where $L_k \to 0$ as $k \to \infty$. Then there exists a subsequence $\left\{ \mathbf{Q}^{L_k} \right\}$ such that $\mathbf{Q}^{L_k} \to \mathbf{Q}^0$ in $W^{1,2}(\Omega, \bar{S}_3)$ as $k \to \infty$, where $\mathbf{Q}^0$ has been defined in (12).

For any compact set $K \subset \bar{\Omega}$ such that K contains no singularity of $\mathbf{Q}^0$, we have that

$$\lim_{L_k \to 0} f_B(\mathbf{Q}^{L_k}(\mathbf{x})) = 0 \quad \mathbf{x} \in K \tag{38}$$

and the limit is uniform on K.

If $\left\{ \mathbf{Q}^{L_k} \right\}$ is a uniaxial small energy sequence, then $\mathbf{Q}^{L_k}$ can be written in the form

$$\mathbf{Q}^{L_k} = s_k \left(\mathbf{n}_k \otimes \mathbf{n}_k - \frac{1}{3} \mathbf{I} \right) \tag{39}$$

for $s_k : \Omega \to \mathbb{R}$ and $n_k \in W^{1,2}(\Omega; S^2)$. Then (38) implies that (up to subsequence), s_k converges uniformly to s_+ everywhere away from S_0 i.e. we have

$$|s_k(\mathbf{x}) - s_+| \leq \epsilon(L_k, \mathbf{x}) \quad \mathbf{x} \in \bar{\Omega} \setminus B_\delta(S_0) \tag{40}$$

where $\epsilon \to 0^+$ as $k \to \infty$, $B_\delta(S_0)$ is a small δ-neighbourhood of the singular set S_0 and $0 < \delta < 1$ is an arbitrary small constant independent of L_k. Similarly, if $\left\{ \mathbf{Q}^{L_k} = s_k \left(\mathbf{n}_k \otimes \mathbf{n}_k - \frac{1}{3} \mathbf{I} \right) + r_k \left(\mathbf{m}_k \otimes \mathbf{m}_k - \frac{1}{3} \mathbf{I} \right) \right\}$ is a biaxial small energy sequence, then (38) implies that

$$|s_+ - s_k| \leq \epsilon_{1,k}, \quad |r_k| \leq \epsilon_{2,k} \tag{41}$$

everywhere away from S_0, where $\epsilon_{1,k}, \epsilon_{2,k} \to 0^+$ as $k \to \infty$.

Uniform convergence in the interior [15]: Let $\left\{ \mathbf{Q}^{L_k} \right\}$ be a small energy sequence in $\mathcal{A}_{\mathbf{Q}}$ such that $L_k \to 0$ as $k \to \infty$. Then (up to a subsequence) $\mathbf{Q}^{L_k} \to \mathbf{Q}^0$ strongly in $W^{1,2}(\Omega, \bar{S})$.

Let $K \subset \Omega$ be a compact set which does not contain any singularities of $\mathbf{Q}^0$. We define

$$e_L(\mathbf{Q}) = \frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{f_B(\mathbf{Q})}{L}.$$

Then
(i) there exists a constant $C > 0$ independent of L such that

$$-\Delta e_L(\mathbf{Q}^L)(\mathbf{x}) \leq C e_L^2 \left(\mathbf{Q}^L\right)(\mathbf{x}) \quad \mathbf{x} \in K \tag{42}$$

for L sufficiently small;
(ii) we have a uniform bound for $e_L(\mathbf{Q}^L)$ in the interior of Ω, away from S_0 in the limit $L \to 0^+$ i.e.

$$e_L(\mathbf{Q}^L)(\mathbf{x}) \leq C^{'}(a^2, b^2, c^2, \Omega) \quad \mathbf{x} \in K \tag{43}$$

for all L sufficiently small and a positive constant $C^{'}$ independent of L;
(iii) $\mathbf{Q}^{L_k}$ converges uniformly to $\mathbf{Q}^0$ everywhere in the interior of Ω, away from S_0.

$$\lim_{k\to\infty} \mathbf{Q}^{L_k}(\mathbf{x}) = \mathbf{Q}^0(\mathbf{x}) \ uniformly\ for\ \mathbf{x} \in K. \tag{44}$$

We emphasize that (43) and (44) only hold in the interior of Ω. In Section 5,6 and 7, we refine these convergence results in the interior and up to the boundary.

5 Uniaxial solutions and their defect sets in $3D$

Let $\mathbf{Q}$ be a uniaxial solution of (26) for a fixed $L > 0$. For $\mathbf{Q}$ uniaxial (of the form $\mathbf{Q} = s(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I})$ where $s : \Omega \to \mathbb{R}$ and $\mathbf{n} \in W^{1,2}(\Omega; S^2)$, see (2)), a direct calculation shows that

$$|\mathbf{Q}|^2 = \frac{2}{3}s^2, \ \mathrm{tr}\mathbf{Q}^3 = \frac{2}{9}s^2$$

$$\left(\mathbf{Q}_{ik}\mathbf{Q}_{kj} - \frac{\delta_{ij}}{3}\mathrm{tr}(\mathbf{Q}^2)\right) = \frac{s}{3}\mathbf{Q}_{ij}$$

and hence, the Euler-Lagrange equations (26) simplify to

$$L\mathbf{Q}_{ij,kk} = \frac{1}{3}\left(2c^2 s^2 - b^2 s - 3a^2\right)\mathbf{Q}_{ij}, \quad i, j = 1 \ldots 3. \tag{45}$$

A uniaxial small energy solution $\mathbf{Q}^L$ is analytic on $\bar{\Omega}$ and is fully characterized by its scalar order parameter s^L and distinguished eigenvector $\mathbf{n}^L$. The scalar order parameter, s^L, is a locally Lipschitz function of $\mathbf{Q}^L$ and hence, is continuous on $\bar{\Omega}$ [27]. From [16], we have that

$$s^L(\mathbf{x}) \leq s_+ \quad \mathbf{x} \in \bar{\Omega} \tag{46}$$

and let $\Theta_L = \left\{\mathbf{x} \in \Omega; s^L(\mathbf{x}) = 0\right\}$ denote the isotropic set of $\mathbf{Q}^L$. We have a topologically non-trivial boundary condition $\mathbf{Q}_b$ in (9) and hence, every interior extension of $\mathbf{Q}_b$ must have discontinuities. We interpret the defect set of $\mathbf{Q}^L$ as being the defect set of $\mathbf{n}^L$. Let $S_{\mathbf{n}}^L$ denote the defect set of $\mathbf{n}^L$ and let $\mathbf{x_n} \in S_{\mathbf{n}}^L$. Then $\mathbf{Q}^L(\mathbf{x_n}) = 0$, since $\mathbf{Q}^L$ is well-defined on $\bar{\Omega}$ and consequently $s^L(\mathbf{x_n}) = 0$. We deduce that $S_{\mathbf{n}}^L \subset \Theta_L$ and from [21], we have that $\mathbf{n}^L$ is analytic everywhere away from Θ_L. We first make an elementary observation about the defect locations, in the vanishing core limit $L \to 0^+$.

Lemma 1 *Let S_0 denote the singular set of the limiting harmonic map $\mathbf{Q}^0$ defined in (12). Let $\mathbf{x_n} \in S_{\mathbf{n}}^L$. Then*

$$dist\,(\mathbf{x_n}, S_0) \leq \epsilon(L)$$

where $\epsilon(L) \to 0$ as $L \to 0^+$.

Proof: Let $\mathbf{x_n} \in S^L_{\mathbf{n}}$. As mentioned above, $s^L(\mathbf{x_n}) = 0$ and $\mathbf{x_n} \in \Theta_L$, where Θ_L has been defined above. However, for a small energy solution, the bulk energy density $f_B(\mathbf{Q}^L)$ converges uniformly to its minimum value, everywhere away from S_0, in the interior and up to the boundary, as $L \to 0$. Recalling (40), we deduce that $dist(\mathbf{x_n}, S_0) \to 0$ as $L \to 0^+$. Lemma 1 now follows. □

Lemma 1 is also equivalent to the statement $dist(\Theta_L, S_0) \to 0$ as $L \to 0^+$ i.e. the isotropic set of a uniaxial small energy sequence converges uniformly to the singular set of a limiting harmonic map in vanishing core limit.

Proposition 1 *Let $\mathbf{Q}^L$ be a uniaxial small energy solution in the admissible space $\mathcal{A}_{\mathbf{Q}}$, for a fixed $L > 0$. Then $\mathbf{Q}^L = s^L\left(\mathbf{n}^L \otimes \mathbf{n}^L - \frac{1}{3}\mathbf{I}\right)$ for some real-valued function $s^L : \overline{\Omega} \to \mathbb{R}^+$ and $\mathbf{n}^L \in W^{1,2}(\Omega; S^2)$. The following equations hold everywhere in Ω, away from the isotropic set Θ_L:*

$$\Delta s^L - 3s^L|\nabla \mathbf{n}^L|^2 = \frac{s^L}{3L}\left(2c^2(s^L)^2 - b^2 s^L - 3a^2\right) \tag{47}$$

$$\Delta \mathbf{n}^L_j + |\nabla \mathbf{n}^L|^2 \mathbf{n}^L_j + 2\frac{\partial_k s^L}{s^L}\mathbf{n}^L_{j,k} = 0 \quad j,k = 1,2,3. \tag{48}$$

Here $\mathbf{n}^L_{j,k}$ denotes the partial derivative $\frac{\partial \mathbf{n}^L_j}{\partial \mathbf{x}_k}$. Alternatively, $\mathbf{n}^L = \left(\sin\theta^L\cos\phi^L, \sin\theta^L\sin\phi^L, \cos\theta^L\right)$, where θ^L, ϕ^L are functions of spherical polar coordinates (r,θ,ϕ) centered at the origin. Then θ^L and ϕ^L satisfy the following coupled nonlinear partial differential equations

$$\nabla \cdot \left((s^L)^2 \nabla \theta^L\right) = (s^L)^2 \sin\theta^L \cos\theta^L |\nabla \phi^L|^2 \tag{49}$$

$$\nabla \cdot \left((s^L)^2 \sin^2\theta^L \nabla \phi^L\right) = 0. \tag{50}$$

Remark: In general, $\mathbf{Q} \in W^{1,2}$ implies that the tensor $\mathbf{n} \otimes \mathbf{n} \in W^{1,2}$. However, for simply-connected three-dimensional domains, $\mathbf{n} \otimes \mathbf{n} \in W^{1,2}(\Omega) \implies \mathbf{n} \in W^{1,2}\left(\Omega; S^2\right)$ [1].

Proof: In what follows, we drop the superscript L from $\mathbf{Q}^L$ for brevity. Since $\mathbf{Q}$ is a classical solution of (45), we have that

$$\mathbf{Q}_{ij,k} = \partial_k s\left(\mathbf{n}_i\mathbf{n}_j - \frac{1}{3}\delta_{ij}\right) + s\left(\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_j\mathbf{n}_{i,k}\right)$$

$$\mathbf{Q}_{ij,kk} = \Delta s\left(\mathbf{n}_i\mathbf{n}_j - \frac{1}{3}\delta_{ij}\right) + 2\partial_k s\left(\mathbf{n}_i\mathbf{n}_{j,k} + \mathbf{n}_j\mathbf{n}_{i,k}\right) + s\left(\mathbf{n}_i\mathbf{n}_{j,kk} + \mathbf{n}_j\mathbf{n}_{i,kk} + 2\mathbf{n}_{i,k}\mathbf{n}_{j,k}\right) \tag{51}$$

where $i,j,k = 1\ldots 3$, $\mathbf{Q}_{ij,k} = \frac{\partial \mathbf{Q}_{ij}}{\partial \mathbf{x}_k}$ etc.

Consider the decoupled equations (45)

$$L\mathbf{Q}_{ij,kk} = \frac{1}{3}\left(2c^2s^2 - b^2 s - 3a^2\right)\mathbf{Q}_{ij}$$

and multiply both sides by $\mathbf{n}_i$ to get the following vector equation

$$\frac{2}{3}\mathbf{n}_j\Delta s + 2\partial_k s\mathbf{n}_{j,k} + s\left(\mathbf{n}_{j,kk} - |\nabla\mathbf{n}|^2\mathbf{n}_j\right) = \frac{2s}{9L}\left(2c^2s^2 - b^2s - 3a^2\right)\mathbf{n}_j. \tag{52}$$

Multiplying both sides of (52) by $\mathbf{n}_j$, we obtain the following scalar equation for s:-

$$\frac{2}{3}\Delta s - 2s|\nabla\mathbf{n}|^2 = \frac{2s}{9L}\left(2c^2s^2 - b^2s - 3a^2\right) \tag{53}$$

and (47) now follows. In (52) and (53), we use (51) and the relations $\mathbf{n}_i\mathbf{n}_i = 1, \mathbf{n}_i\mathbf{n}_{i,k} = 0$ and $\mathbf{n}_i\mathbf{n}_{i,kk} = -|\nabla\mathbf{n}|^2$.

For (48), we multiply both sides of the vector equation (52) by the derivative $\mathbf{n}_{j,p}$ for $p = 1, 2, 3$ to get the following system of three equations -

$$2\partial_k s\mathbf{n}_{j,p}\mathbf{n}_{j,k} + s\mathbf{n}_{j,p}\mathbf{n}_{j,kk} = 0 \quad p = 1, 2, 3. \tag{54}$$

Multiplying both sides by the scalar order parameter s, (54) simplifies to

$$\mathbf{n}_{j,p}\partial_k\left(s^2\mathbf{n}_{j,k}\right) = 0 \quad p = 1, 2, 3. \tag{55}$$

Next, we note that for a fixed p, $(\mathbf{n}_j, \mathbf{n}_{j,p}, \mathbf{e}_j)$ form an orthogonal basis at each point $\mathbf{x} \in \Omega$ (where $\mathbf{e}_j = \mathbf{n}_j \times \mathbf{n}_{j,p}$), away from the isotropic set Θ_L so that

$$\partial_k\left(s^2\mathbf{n}_{j,k}\right) = \lambda_1\mathbf{n}_j + \lambda_2\mathbf{e}_j \tag{56}$$

where

$$\lambda_1 = \mathbf{n}_j\partial_k\left(s^2\mathbf{n}_{j,k}\right) = -s^2|\nabla\mathbf{n}|^2.$$

We substitute (56) into (52) to get

$$\frac{2s}{3}\mathbf{n}_j\Delta s - 2s^2|\nabla\mathbf{n}|^2\mathbf{n}_j + \lambda_2\mathbf{e}_j = \frac{2s^2}{9L}\left(2c^2s^2 - b^2s - 3a^2\right)\mathbf{n}_j$$

from which we deduce that $\lambda_2 = 0$. Hence

$$\partial_k\left(s^2\mathbf{n}_{j,k}\right) + s^2|\nabla\mathbf{n}|^2\mathbf{n}_j = 0 \quad j = 1\ldots 3 \tag{57}$$

from which (48) follows.

An alternative formulation of (55) can be obtained by writing the unit-vector field $\mathbf{n}$ in terms of its spherical angles, $\theta^L(r,\theta,\phi)$ and $\phi^L(r,\theta,\phi)$, where (r,θ,ϕ) are spherical polar coordinates centered at the origin i.e.

$$\mathbf{n} = \left(\sin\theta^L\cos\phi^L, \sin\theta^L\sin\phi^L, \cos\theta^L\right). \tag{58}$$

Straightforward computations show that

$$\frac{\partial\mathbf{n}}{\partial\mathbf{x}_k} = \partial_k\theta^L\left(\cos\theta^L\cos\phi^L, \cos\theta^L\sin\phi^L, -\sin\theta^L\right) + \sin\theta^L\ \partial_k\phi^L\left(-\sin\phi^L, \cos\phi^L, 0\right)$$

$$\frac{\partial^2\mathbf{n}}{\partial\mathbf{x}_k\partial\mathbf{x}_k} = \partial_{kk}\theta^L\left(\cos\theta^L\cos\phi^L, \cos\theta^L\sin\phi^L, -\sin\theta^L\right) - \left(\partial_k\theta^L\right)^2\left(\sin\theta^L\cos\phi^L, \sin\theta^L\sin\phi^L, \cos\theta^L\right) +$$

$$+2\cos\theta^L\partial_k\theta^L\partial_k\phi^L\left(-\sin\phi^L, \cos\phi^L, 0\right) + \sin\theta^L\partial_{kk}\phi^L\left(-\sin\phi^L, \cos\phi^L, 0\right) - \sin\theta^L\left(\partial_k\phi^L\right)^2\left(\cos\phi^L, \sin\right.$$

Substituting (59) into (52) and taking the dot product of both sides with $(\cos\theta^L\cos\phi^L, \cos\theta^L\sin\phi^L, -\sin$ we obtain

$$2\partial_k s\partial_k\theta^L + s\partial_{kk}\theta^L - s\sin\theta^L\cos\theta^L|\nabla\phi^L|^2 = 0. \tag{60}$$

We multiply both sides of (60) by s and equation (49) now follows. Similarly, we take the scalar product of (52) with the unit-vector $\left(-\sin\phi^L, \cos\phi^L, 0\right)$ to obtain

$$s\sin\theta^L\partial_{kk}\phi^L + 2s\cos\theta^L\partial_k\theta^L\partial_k\phi^L + 2\sin\theta^L\partial_k s\partial_k\phi^L = 0. \tag{61}$$

As above, we multiply both sides of (61) by $s \sin \theta^L$ and (50) then follows. The proof of Proposition 1 is now complete. □

Comment: We note that for s constant, (48) is equivalent to the harmonic map equations $\Delta \mathbf{n}_0 + |\nabla \mathbf{n}_0|^2 \mathbf{n}_0 = 0$ *[5].*

Next, we use asymptotic methods to predict the minimizer profile near isolated isotropic points in Θ_L and establish a $1-1$ correspondence between isolated isotropic points and isolated point defects.

Proposition 2 *Let* $\mathbf{Q}^L$ *be a uniaxial small energy solution in the admissible space* $\mathcal{A}_{\mathbf{Q}}$*, for a fixed* $L > 0$*. Then* $\mathbf{Q}^L(\mathbf{x}) = s^L(\mathbf{x}) \left(\mathbf{n}^L(\mathbf{x}) \otimes \mathbf{n}^L(\mathbf{x}) - \frac{1}{3}\mathbf{I} \right)$*. Let* $\Gamma_{\mathbf{n}} \subset \Omega$ *denote the set of isolated point defects in* $\mathbf{n}^L$ *and let* $\Gamma_L \subset \Omega$ *denote the set of isolated isotropic points of* $\mathbf{Q}^L$*.*

(i) Let $\mathbf{x}_L \in \Gamma_L$ *be an isolated interior isotropic point. Let* (r, θ, ϕ) *denote a local spherical co-ordinate system centered at* $\mathbf{x}_L$*;, then*

$$\left| \nabla \mathbf{n}^L \right|^2 \sim \frac{\alpha(\theta, \phi)}{r^2} \qquad as\ r \to 0 \tag{62}$$

where α *only depends on* θ, ϕ *and is independent of the radial coordinate* r*. Then* $\mathbf{x}_L \in \Gamma_{\mathbf{n}}$ *too.*
(ii) Let $\mathbf{x}_{\mathbf{n}} \in \Gamma_{\mathbf{n}}$ *be an isolated point defect. Then* $\mathbf{x}_{\mathbf{n}} \in \Gamma_L$ *and hence,* $\Gamma_{\mathbf{n}} = \Gamma_L$*.*

Proof: (i) Consider the coupled equation (47):

$$\Delta s - 3s|\nabla \mathbf{n}|^2 = \frac{s}{3L}\left(2c^2 s^2 - b^2 s - 3a^2\right) \tag{63}$$

Let $\mathbf{x}_L \in \Gamma_L$ be an isolated isotropic point. Since $s^L(\mathbf{x}) = \frac{3}{2}\mathbf{Q}^L(\mathbf{x}) \left(\mathbf{n}^L(\mathbf{x}) \otimes \mathbf{n}^L(\mathbf{x}) - \frac{1}{3}\mathbf{I} \right)$ is the product of two analytic matrices away from $\mathbf{x}_L$, we deduce that $s^L(\mathbf{x})$ is analytic for $0 < r < r_0$, for some $r_0 > 0$. We are interested in the leading-order behaviour of $|\nabla \mathbf{n}^L|^2$ as $r \to 0$.

From the local analyticity of s^L, we have the following power series expansion

$$s^L(\mathbf{x}) = r^n g(\theta, \phi) + h\left(r, \theta, \phi\right) \quad 0 < r < r_b < r_0,\ n \geq 1, \tag{64}$$

where (r, θ, ϕ) is a local spherical coordinate system centered at $\mathbf{x}_L$, $\left|\frac{h}{r^n g}\right| = o(1)$ as $r \to 0$ and r_b is the radius of convergence of the series (64). Further, $g \neq 0$ for $r \neq 0$ and $\{g, h\}$ are analytic functions with bounded derivatives in a sufficiently small neighbourhood of $\mathbf{x}_L$. Substituting (64) into (63) and expressing Δs^L in spherical polar coordinates

$$\Delta s^L = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial s^L}{\partial r}\right) + \frac{1}{r^2 \sin^2 \phi}\frac{\partial^2 s^L}{\partial \theta^2} + \frac{1}{r^2 \sin \phi}\frac{\partial}{\partial \phi}\left(\sin \phi \frac{\partial s^L}{\partial \phi}\right), \tag{65}$$

we have that

$$\begin{aligned}
& r^{n-2}\left[n(n+1)g + \frac{g_{\theta\theta}}{\sin^2 \phi} + g_{\phi\phi} + \cot \phi g_\phi \right] + \\
& + \frac{2h_r}{r} + h_{rr} + \frac{h_{\theta\theta}}{r^2 \sin^2 \phi} + \frac{h_{\phi\phi}}{r^2} + \cot \phi \frac{h_\phi}{r^2} - \\
& - 3|\nabla \mathbf{n}^L|^2 \left(r^n g(\theta, \phi) + h(r, \theta, \phi)\right) = \\
& = \frac{(r^n g + h)}{3L}\left[2c^2 \left(r^n\ g + h\right)^2 - b^2 \left(r^n\ g + h\right) - 3a^2\right] \quad as\ r \to 0.
\end{aligned} \tag{66}$$

All the terms on the right-hand side are $O(r^n)$ whereas the leading order term on the left-hand side of (66) is $O(r^{n-2})$. Since h is an analytic function and $\left|\frac{h}{r^n}\right| = o(1)$ as $r \to 0$, we have that $h_r/r, h_{rr} = o(r^{n-2})$ as $r \to 0$. Therefore, for (66) to hold as $r \to 0$, we must have

$$|\nabla \mathbf{n}^L|^2 \sim \frac{1}{3r^2}\left[n(n+1) + \frac{g_{\theta\theta}}{g\sin^2\phi} + \frac{g_{\phi\phi}}{g} + \cot\phi \frac{g_\phi}{g}\right] \quad as\ r \to 0 \tag{67}$$

and (62) now follows. It follows that $|\nabla \mathbf{n}^L|^2$ is not defined as $r \to 0$ and hence, the isolated isotropic point $\mathbf{x}_L \in \Gamma_{\mathbf{n}}$ too.
(ii) Let $\mathbf{x}_{\mathbf{n}} \in \Gamma_{\mathbf{n}}$. Then $\mathbf{Q}^L(\mathbf{x}_{\mathbf{n}}) = 0$, since $\mathbf{Q}^L$ is well-defined on $\bar{\Omega}$. Therefore, we must have $s^L(\mathbf{x}_{\mathbf{n}}) = 0$ and by definition, $\mathbf{x}_{\mathbf{n}} \in \Gamma_L$. Combining (i) and (ii), we conclude that $\Gamma_L = \Gamma_{\mathbf{n}}$. $\Box$

Comment: We briefly comment on the relevance of Propositions 1 and 2 to uniaxial Landau-de Gennes minimizers (if they exist). In [18], the authors study minimizers, $\mathbf{u}$*, of the Ginzburg-Landau functional on* $\mathbb{R}^3$ *with* $deg(\mathbf{u}) = 1$ *at* ∞ *and demonstrate that every local minimizer has the "radial-hedgehog" structure* $\frac{\mathbf{r}}{|\mathbf{r}|}$*, modulo a rotation i.e. these local minimizers support an isolated point defect in the interior. The vanishing core limit is equivalent to studying Landau-de Gennes minimizers on the whole Euclidean space* $\mathbb{R}^3$*. By analogy with the results in [18], one might expect that in the vanishing core limit, uniaxial Landau-de Gennes minimizers can only account for isolated point defects and all higher-dimensional defects are intrinsically biaxial.*
We hypothesize that $n = 2$ *in (64) i.e. we have a quadratic decay of the scalar order parameter as we approach point defects, by analogy with the study of vortices in Ginzburg-Landau theory [17].*
We note that the estimate (62) is analogous to a similar result on singularity profiles within the Oseen-Frank theory of uniaxial nematic liquid crystals with a constant scalar order parameter s *[5]. Let* $\mathbf{n}$ *be a global minimizer of the Dirichlet energy (13) in the admissible space* $\mathcal{A}_{\mathbf{n}}$ *in (14). In [5], the authors show that near every singularity* $\mathbf{x}_p \in \Omega$*, we have*

$$\mathbf{n} \sim R\frac{\mathbf{x} - \mathbf{x}_p}{|\mathbf{x} - \mathbf{x}_p|} \tag{68}$$

for some rotation $R \in SO(3)$*. Therefore ,*

$$|\nabla \mathbf{n}|^2 \sim \frac{2}{|\mathbf{x} - \mathbf{x}_p|^2} \quad as\ \mathbf{x} \to \mathbf{x}_p.$$

The estimate (62) suggests that we have a similar radial hedgehog-type of profile (68) near the isolated zero $\mathbf{x}_L \in \Omega$*, for uniaxial Landau-de Gennes minimizers.*

6 Far-field results

In this section, we study the qualitative properties of uniaxial small energy solutions $\{\mathbf{Q}^L\}$ away from the isotropic set Θ_L, in the vanishing core limit, $L \to 0$. From Lemma 1, this is equivalent to studying the qualitative properties of $\{\mathbf{Q}^L\}$ away from the singular set S_0 of the limiting harmonic map $\mathbf{Q}^0$ defined in (12), as $L \to 0^+$.

Let $\mathbf{Q}^L = s^L\left(\mathbf{n}^L \otimes \mathbf{n}^L - \frac{1}{3}\mathbf{I}\right)$ be a uniaxial small energy solution of (26), for fixed $L > 0$. Recall that for L sufficiently small,

$$0 \le s_+ - s^L(\mathbf{x}) \le \epsilon_1(L) \tag{69}$$

or equivalently

$$\left||\mathbf{Q}^L|^2 - \frac{2}{3}s_+^2\right| \le \epsilon_2(L) \tag{70}$$

where $\epsilon_1(L), \epsilon_2(L) \to 0$ as $L \to 0^+$, everywhere away from S_0.

Our first result is an inequality for

$$A^L = \frac{1}{2}\mathbf{Q}^L_{ij,k}\mathbf{Q}^L_{ij,k}$$

that holds everywhere away from S_0 on $\bar{\Omega}$. We do not use Lemma 2 in the subsequent sections but keep it as an interesting technical result.

Lemma 2 *Let $A^L = \frac{1}{2}\mathbf{Q}^L_{ij,k}\mathbf{Q}^L_{ij,k}$ by definition. Then we have the following inequality on $\Omega \setminus B_\delta(S_0)$ for L sufficiently small*

$$-\Delta A^L + \left|\nabla^2 \mathbf{Q}^L\right|^2 \leq \frac{1}{\alpha^2}\left|\nabla^2 \mathbf{Q}^L\right|^2 + \alpha^4 \frac{{A^L}^2}{|\mathbf{Q}^L|^2} \tag{71}$$

where $\alpha > 1$ is a positive constant independent of L that can be worked out explicitly, $B_\delta(S_0)$ is a small δ-neighbourhood of S_0 and $\delta > 0$ is independent of L.

Proof: The derivation of (71) closely follows the methods in [4]. In what follows, we drop the superscript L for brevity. First, consider the decoupled equations (45); setting

$$f(s) = \left(2c^2 s^2 - b^2 s - 3a^2\right)$$

and differentiating both sides of (45) with respect to $\mathbf{x}_p$, we obtain

$$\mathbf{Q}_{ij,kkp} = \frac{\mathbf{Q}_{ij,p}}{3L} f(s) + f^{'}(s)\frac{\mathbf{Q}_{ij}}{\sqrt{6}L}\frac{\mathbf{Q}_{rs}\mathbf{Q}_{rs,p}}{|\mathbf{Q}|} \ for\ p = 1,2,3. \tag{72}$$

From (70) and the global upper bound (31), we have that $|\mathbf{Q}|$ is bounded away from zero on $\Omega \setminus B_\delta(S_0)$ and

$$\begin{aligned} & f(s) \leq 0 \\ & f^{'}(s) > 0 \\ & f^{''}(s) > 0, \end{aligned} \tag{73}$$

on the set $\Omega \setminus B_\delta(S_0)$, where $f^{'}(s) = \frac{df}{ds}$, $f^{''}(s) = \frac{d^2 f}{ds^2}$ etc. A straightforward computation shows that

$$\Delta A = |\nabla^2 \mathbf{Q}|^2 + \mathbf{Q}_{ij,k}\mathbf{Q}_{ij,ppk} \tag{74}$$

(where $|\nabla^2 \mathbf{Q}|^2 = \mathbf{Q}_{ij,kp}\mathbf{Q}_{ij,kp}$) and using (72), we obtain

$$\Delta A = |\nabla^2 \mathbf{Q}|^2 + |\nabla \mathbf{Q}|^2 \frac{f(s)}{3L} + \frac{f^{'}(s)}{\sqrt{6}L}\frac{(\mathbf{Q}\cdot\nabla\mathbf{Q})^2}{|\mathbf{Q}|}. \tag{75}$$

Note that $(\mathbf{Q}\cdot\nabla\mathbf{Q})^2 = \frac{1}{4}\left|\nabla|\mathbf{Q}|^2\right|^2$. From (73) and (45), we have the following inequality

$$-\Delta A + |\nabla^2 \mathbf{Q}|^2 \leq |\nabla \mathbf{Q}|^2 \frac{|\Delta \mathbf{Q}|}{|\mathbf{Q}|}. \tag{76}$$

Finally, we use the inequality

$$|\Delta \mathbf{Q}| \leq \alpha \left|\nabla^2 \mathbf{Q}\right|$$

where $\alpha > 1$ is a positive constant that can be worked out explicitly. Substituting the above into (76),

$$-\Delta A + |\nabla^2 \mathbf{Q}|^2 \leq 2\alpha A \frac{|\nabla^2 \mathbf{Q}|}{|\mathbf{Q}|} \leq \frac{1}{\alpha^2}|\nabla^2 \mathbf{Q}|^2 + \alpha^4 \frac{A^2}{|\mathbf{Q}|^2} \tag{77}$$

and (71) now follows. □

We recall the uniform convergence result in (44) and (43), whereby we establish a uniform bound for $|\nabla \mathbf{Q}^L|$, independent of L, everywhere away from S_0 in the interior of Ω. The next step is to extend this uniform convergence result up to the boundary. To do so, we adapt the small energy regularity theorem in [7] to the Landau-de Gennes framework to obtain a uniform bound for $|\nabla \mathbf{Q}^L|$ independent of L, everywhere away from S_0 up to the boundary.

Consider a boundary point $\mathbf{x}_0 \in \partial\Omega$ and define the region $\Omega_r(\mathbf{x}_0) = \bar{\Omega} \cap B_r(\mathbf{x}_0)$, where $B_r(\mathbf{x}_0)$ is a ball of radius r centered at $\mathbf{x}_0$. Let ρ be a suitably small positive constant such that for any $\mathbf{x}_0 \in \partial\Omega$, we may choose a coordinate system $\{\mathbf{x}_\alpha\}$ so that $\mathbf{x}_0$ is at the origin and $\Omega_\rho(\mathbf{x}_0)$ corresponds to $B_\rho^+(\mathbf{x}_0) = \left\{\mathbf{x} \in \bar{\Omega}; |\mathbf{x}| \leq \rho;\ x_3 \geq 0\right\}$.

Proposition 3 *Let $\left\{\mathbf{Q}^{L_k}\right\}$ be a uniaxial small energy sequence in the admissible space $\mathcal{A}_{\mathbf{Q}}$, where $L_k \to 0$ as $k \to \infty$. We can extract a subsequence such that $\mathbf{Q}^{L_k} \to \mathbf{Q}^0$ strongly in $W^{1,2}(\Omega; \bar{S}_3)$ as $k \to \infty$. Let $\mathbf{x}_0 \in \partial\Omega$ be such that $\Omega_r(\mathbf{x}_0)$ contains no singularity of the limiting harmonic map $\mathbf{Q}^0$. Then there exists $C_1 > 0, C_2 > 0, r_0 > 0, \bar{L}_0 > 0$ (all constants independent of L_k) so that if*

$$\int_{\Omega_r(\mathbf{x}_0)} \frac{1}{2}|\nabla \mathbf{Q}^L|^2 + \frac{f_B(\mathbf{Q}^L)}{L}\, d\mathbf{x} \leq C_1 \quad r < \min\{r_0, \rho\} \tag{78}$$

then

$$r^2 \sup_{\Omega_{r/2}(\mathbf{x}_0)} e_L(\mathbf{Q}^L) \leq C_2 \quad \text{for all } L < \bar{L}_0 \tag{79}$$

where

$$e_L(\mathbf{Q}^L) = \frac{1}{2}|\nabla \mathbf{Q}^L|^2 + \frac{f_B(\mathbf{Q}^L)}{L}.$$

Proof: The first half of the proof of Proposition 3 closely follows the scaling arguments for the interior uniform convergence result (43) in [15] and the second half closely follows the arguments in Theorem 2.1 in [7].

We first recall from (38) that since $\Omega_r(\mathbf{x}_0)$ contains no singularity of $\mathbf{Q}^0$, $\exists \mathbf{m}(\mathbf{x}) \in S^2$ such that

$$\left|\mathbf{Q}^L(\mathbf{x}) - s_+\left(\mathbf{m}(\mathbf{x}) \otimes \mathbf{m}(\mathbf{x}) - \frac{1}{3}\mathbf{I}\right)\right| < \epsilon_0 << 1 \quad \mathbf{x} \in \Omega_r(\mathbf{x}_0) \tag{80}$$

for L sufficiently small. We also note that $\mathbf{Q}^0$ has a finite number of interior isolated point defects and therefore, for every $\mathbf{x}_0 \in \partial\Omega$, we can define $\Omega_r(\mathbf{x}_0)$ for some $r > 0$ sufficiently small such that $\Omega_r(\mathbf{x}_0)$ contains no singularity of $\mathbf{Q}^0$.

We continue reasoning similarly to [15]. We fix an arbitrary $L_k < \bar{L}_0$. We let $0 < r_1 < \frac{2r}{3} < \min\left\{\frac{2r_0}{3}, \frac{2\rho}{3}\right\}$ and $\mathbf{x}_1 \in \Omega_{r_1}(\mathbf{x}_0)$ be such that

$$\max_{0 \leq s \leq \frac{2r}{3}} \left(\frac{2r}{3} - s\right)^2 \max_{\Omega_s(\mathbf{x}_0)} e_{L_k}\left(\mathbf{Q}^{L_k}\right) = \left(\frac{2r}{3} - r_1\right)^2 e_{L_k}\left(\mathbf{Q}^{L_k}\right)(\mathbf{x}_1). \tag{81}$$

Define $e_1^{L_k} = \max_{\mathbf{x}\in\Omega_{r_1}(\mathbf{x}_0)} e_{L_k}(\mathbf{Q}^{L_k}) = e_{L_k}(\mathbf{Q}^{L_k})(\mathbf{x}_1)$. Then

$$\max_{\Omega_{\frac{2/3r-r_1}{2}}(\mathbf{x}_1)} e_{L_k}(\mathbf{Q}^{L_k}) \leq 4e_1^{L_k} \tag{82}$$

where we use the inclusion $\Omega_{\frac{2/3r-r_1}{2}}(\mathbf{x}_1) \subset \Omega_{\frac{2/3r+r_1}{2}}(\mathbf{x}_0)$, $\frac{2/3r+r_1}{2} \leq \frac{2r}{3}$ by definition of r_1 and the inequalities (81).

Define $r_2 = \frac{2/3r-r_1}{2}\sqrt{e_1^{L_k}}$ and let

$$\mathbf{R}^{L_k}(\mathbf{x}) = \mathbf{Q}^{L_k}\left(\mathbf{x}_1 + \frac{\mathbf{x}}{\sqrt{e_1^{L_k}}}\right). \tag{83}$$

Let $\bar{L}_k = e_1^{L_k} L_k$. Then $\mathbf{R}^{L_k}$ has the following properties on $\Omega_{r_2}(0)$:-

$$e_{\bar{L}_k}(\mathbf{R}^{L_k}) = \frac{1}{e_1^{L_k}} e_{L_k}(\mathbf{Q}^{L_k}) \tag{84}$$

$$\max_{\mathbf{x}\in\Omega_{r_2}(0)} e_{\bar{L}_k}(\mathbf{R}^{L_k}) \leq 4 \quad e_{\bar{L}_k}(\mathbf{R}^{L_k})(0) = 1 \tag{85}$$

$$\mathbf{R}^{L_k}_{ij,kk} = \frac{1}{\bar{L}_k}\left(2c^2s^2 - b^2s - 3a^2\right)\mathbf{R}^{L_k}_{ij} \tag{86}$$

where $s^2 = \frac{3}{2}\left|\mathbf{Q}^{L_k}\right|^2$.

We next claim that $r_2 \leq 1$. It is obvious that $r_2 \leq 1$ implies the conclusion (79). We prove this claim by contradiction. Assume that $r_2 > 1$; then using the same arguments as in [7], one is led to the existence of a sequence of solutions $\left\{\mathbf{R}^{L_k}\right\}$ of (86) on $\Omega_1(0) = B_1^+(0)$, with the following properties: -

$$\begin{aligned}
&-\Delta\mathbf{R}^{L_k}_{ij} + \frac{1}{\bar{L}_k}\left(2c^2s^2 - b^2s - 3a^2\right)\mathbf{R}^{L_k}_{ij} = 0 \ in\ B_1^+(0) \\
&\max_{\mathbf{x}\in B_1^+(0)} e_{\bar{L}_k}(\mathbf{R}^{L_k}) \leq 4 \quad e_{\bar{L}_k}(\mathbf{R}^{L_k})(0) = 1 \\
&\mathbf{R}^{L_k}|_{\mathbf{x}_3=0} = \mathbf{Q}_b\left(\mathbf{x}_1 + \frac{\mathbf{x}}{\sqrt{e_1^{L_k}}}\right) \ with \\
&|\nabla\mathbf{R}^{L_k}||_{\mathbf{x}_3=0} \leq \epsilon_k||\nabla\mathbf{Q}_b||_{L^\infty(\partial\Omega)},\ |\nabla^2\mathbf{R}^{L_k}||_{\mathbf{x}_3=0} \leq \epsilon_k^2||\nabla^2\mathbf{Q}_b||_{L^\infty(\partial\Omega)} \ with\ \epsilon_k \to 0\ as\ k \to \infty \\
&\int_{B_1^+(0)} e_{\bar{L}_k}(\mathbf{R}^{L_k})\, d\mathbf{x} \leq \delta_k \to 0^+ \ as\ k \to \infty.
\end{aligned} \tag{87}$$

From (42) and (85), we deduce that $\mathbf{R}^{L_k}$ satisfies the following Bochner-type inequality on $B_1^+(0)$:-

$$-\Delta e_{\bar{L}_k}(\mathbf{R}^{L_k}) \leq C' e_{\bar{L}_k}(\mathbf{R}^{L_k}) \quad \mathbf{x} \in B_1^+(0) \tag{88}$$

where C' is a constant independent of L_k.

Next, we write $\mathbf{R}^{L_k}$ explicitly in terms of its scalar order parameter and leading eigenvector -

$$\mathbf{R}^{L_k}_{ij} = s_k\left(\mathbf{n}^k_i\mathbf{n}^k_j - \frac{1}{3}\delta_{ij}\right) \quad \mathbf{n}^k \in W^{1,2}\left(\Omega; S^2\right) \tag{89}$$

where $|\mathbf{R}^{L_k}|^2 = \frac{2}{3}s_k^2$ and

$$|s_k - s_+| \leq \frac{s_+}{100}$$

from (80), for k sufficiently large. From Proposition 1, we have that s_k and $\mathbf{n}^k$ satisfy the following equations in $B_1^+(0)$:-

$$\Delta s_k - 3s_k|\nabla \mathbf{n}^k|^2 = \frac{s_k}{3\bar{L}_k}(2c^2 s_k^2 - b^2 s_k - 3a^2) \tag{90}$$

$$\Delta \mathbf{n}_j^k + |\nabla \mathbf{n}^k|^2 \mathbf{n}_j^k + 2\frac{\partial_p s_k}{s_k}\mathbf{n}_{j,p}^k = 0 \tag{91}$$

$$|\nabla \mathbf{R}^{L_k}|^2 = \frac{2}{3}|\nabla s_k|^2 + 2s_k^2|\nabla \mathbf{n}^k|^2 \leq 4. \tag{92}$$

From (80) and (92), we deduce that

$$|\nabla \mathbf{n}^k| \leq \frac{2}{s_+}, \quad \left|\frac{2\nabla s_k}{s_k}\right| \leq \frac{6}{s_+} \quad \textit{on } B_1^+(0). \tag{93}$$

We combine (93) and (91) to deduce that

$$\sup_{B_{2/3}^+(0)} |\nabla \mathbf{n}^k|^2 \leq c\delta_k^{1/3} \to 0 \quad k \to \infty \tag{94}$$

where c is a constant independent of k. In particular, this implies that $||\nabla \mathbf{n}^k||_{L^\infty(\partial\Omega)} \leq c\delta_k^{1/3} \to 0$ as $k \to \infty$. The proof of (94) is identical to the proof of Theorem 2.1 in [7] and the details are omitted for brevity.

Next, look at the equation (47) and introduce the function

$$\bar{s}_k = s_+ - s_k.$$

Then $\bar{s}_k$ is a solution of the following problem on $B_1^+(0)$:-

$$-\Delta \bar{s}_k = 3s_k|\nabla \mathbf{n}^k|^2 - \frac{2c^2 s_k \bar{s}_k (s_k - s_-)}{3\bar{L}_k}$$
$$\bar{s}_k(\mathbf{x}) = 0 \quad \mathbf{x} \in \left\{B_1^+(0) \cap x_3 = 0\right\} \tag{95}$$

where $s_- < 0$ is a constant. Repeating the same arguments as in [7], we obtain the following estimates:-

$$\bar{s}_k(\mathbf{x}) \leq c_1 x_3 \delta_k^{1/3} \quad \mathbf{x} \in B_{1/2}^+(0)$$
$$||\nabla \bar{s}_k||_{L^\infty(\partial\Omega)} = ||\nabla s_k||_{L^\infty(\partial\Omega)} \leq c_0\delta_k^{1/3} \to 0 \quad k \to \infty \tag{96}$$

where c_0 and c_1 are positive constants independent of L_k.

Finally, we define $\tilde{e}_k = \max\left\{0, e_{L_k}(\mathbf{R}^{L_k}) - (c + c_0)\delta_k^{1/3}\right\}$. (Recall that $f_B(\mathbf{R}^{L_k}) = 0$ on $x_3 = 0$ because of the choice of the boundary condition $\mathbf{Q}_b$.) Then from (42), (94) and (96), we have that

$$-\Delta \tilde{e}_k(\mathbf{x}) \leq C'' \tilde{e}_k(\mathbf{x}) \quad \mathbf{x} \in B_{1/2}^+(0)$$
$$\tilde{e}_k(\mathbf{x})|_{x_3=0} = 0 \tag{97}$$

for a constant $C^{''}$ independent of L_k. Using standard arguments as in [7], (97) implies that

$$\sup_{\mathbf{x}\in B^+_{1/4}(0)} \tilde{e}_k(\mathbf{x}) \leq c_3\delta_k \to 0^+ \textit{ as } k\to\infty$$

contradicting (85). The proof of Proposition 3 is now complete. □

For the reader's convenience, we quote Lemma 2 from [4] which is used in Proposition 4:

Lemma 2 from [4]: Let $\omega(r)$ be a solution of

$$\begin{aligned} -\epsilon^2\Delta\omega + \omega = 0 \textit{ on } B(0,R) \\ \omega = 1 \textit{ on } \partial B(0,R). \end{aligned} \tag{98}$$

Then for $\epsilon < \frac{3R}{4}, \omega(r) \leq e^{\frac{1}{4\epsilon R}\left(r^2-R^2\right)}$ on $B(0,R)$.

Proposition 4 *Let $\left\{\mathbf{Q}^{L_k}\right\}$ be a uniaxial small energy sequence of solutions of (26) in admissible space $\mathcal{A}_{\mathbf{Q}}$, where $L_k\to 0^+$ as $k\to\infty$. Then as $k\to\infty$, we can extract a suitable subsequence such that $\mathbf{Q}^{L_k}\to\mathbf{Q}^0$ in $C^{1,\alpha}\left(\overline{\Omega}\setminus B_\delta(S_0)\right)$ for some $0<\alpha<1$ and $B_\delta(S_0)$ is a small δ-neighbourhood of the singular set, S_0, of the limiting harmonic map, $\mathbf{Q}^0$, where $\mathbf{Q}^0$ has been defined in (12) and δ is independent of L_k.*

Proof: The proof follows the methods in [4] and the key ingredient is to establish a global bound for $\frac{s_+ - s^{L_k}}{L_k}$, everywhere away from S_0, for L_k sufficiently small.

We drop the superscript L_k in what follows for convenience. Consider the equation (47) on $\overline{\Omega}\setminus B_\delta(S_0)$ and introduce the function

$$\psi = \frac{s_+ - s}{L}, \tag{99}$$

s_+ has been defined in (29) and $s_- = \left(b^2 - \sqrt{b^2+24a^2c^2}\right)/4c^2 < 0$. Then (47) can be re-written as

$$\Delta s - 3s|\nabla\mathbf{n}|^2 = -\frac{2c^2 s}{3}\psi\left(s - s_-\right) \tag{100}$$

From (31) and (40), we have that $\frac{2}{3}s_+^2 \geq |\mathbf{Q}|^2 \geq \frac{2}{3}s_+^2 - \epsilon_L$ where $\epsilon_L\to 0$ as $L\to 0$, on $\overline{\Omega}\setminus B_\delta(S_0)$. Therefore,

$$\frac{2c^2 s}{3}\left(s - s_-\right) \geq \frac{1}{\beta}$$

on $\overline{\Omega}\setminus B_\delta(S_0)$, where β is a positive constant independent of L.

We note that $|\nabla\mathbf{Q}|^2 = \frac{2}{3}|\nabla s|^2 + 2s^2|\nabla\mathbf{n}|^2$ where $\mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right)$. We recall the global uniform bound (79) everywhere away from S_0 to deduce that

$$|\nabla\mathbf{n}|^2 \leq C(a^2,b^2,c^2,\Omega)$$

on $\overline{\Omega}\setminus B_\delta(S_0)$. Combining the above, we have that ψ satisfies the following inequality on $\overline{\Omega}\setminus B_\delta(S_0)$

$$-\beta L\Delta\psi + \psi \leq \gamma|\nabla\mathbf{n}|^2 \leq D(a^2,b^2,c^2,\Omega) \tag{101}$$

where γ and D are positive constants independent of L. Applying standard maximum principle arguments, we conclude that

$$\|\psi\|_{L^\infty(\Omega\setminus B_\delta(S_0))} \leq D^{'}(a^2,b^2,c^2,\Omega) \tag{102}$$

where $D^{'}$ is a positive constant independent of L.

Consider the governing equations (45) for a uniaxial global minimizer $\mathbf{Q}$; they can be written in terms of the function ψ as shown below -

$$\Delta \mathbf{Q} = \frac{1}{3L}\left(2c^2 s^2 - b^2 s - 3a^2\right)\mathbf{Q} \leq -\alpha\psi\mathbf{Q} \tag{103}$$

where $\alpha > 0$ is a constant independent of L, we have used the definition of ψ in (99) and the uniform convergence of bulk energy density everywhere away from S_0 (refer to (38)). Finally, we combine the global upper bound (31) and the L^∞-estimate (102) to conclude that

$$\|\Delta \mathbf{Q}\|_{L^\infty(\bar{\Omega}\setminus B_\delta(S_0))} \leq D^{''}(a^2, b^2, c^2, \Omega) \tag{104}$$

where $D^{''}$ is a positive constant independent of L i.e. $|\Delta \mathbf{Q}|$ can be bounded independently of L_k everywhere away from S_0. Finally, we use (104) and Sobolev estimates to establish $\left\{\mathbf{Q}^{L_k}\right\} \to \mathbf{Q}^0$ in $C^{1,\alpha}(\bar{\Omega}\setminus B_\delta(S_0))$ as $k\to\infty$, for some $0<\alpha<1$. The proof of Proposition 4 is now complete. $\Box$

Comment: One immediate consequence of (102) is that $s_+ - s^L \leq CL$, *where* C *is a positive constant independent of* L, *everywhere away from* S_0 *in the limit* $L \to 0$. *This explicitly estimates the rate of convergence in (40) and improves upon a previous estimate in [15] where an analysis of the bulk energy density* f_B *in (5) shows that* $s_+ - s \leq C_1\sqrt{L}$ *where* C_1 *is a positive constant independent of* L.

Comment: Motivated by Proposition 4, one might define the defect set of a uniaxial small energy solution to be (see [12] for a similar definition in the Oseen-Frank theory of uniaxial nematics with constant order parameter)

$$\Phi = \left\{\mathbf{x}\in\bar{\Omega};\ \lim_{r\to 0}\int_{\bar{\Omega}\cap B(\mathbf{x},r)} \frac{1}{2}|\nabla \mathbf{Q}|^2 + \frac{f_B(\mathbf{Q})}{L}\, dV > 0\right\}. \tag{105}$$

Lemma 3 *Let* $\mathbf{Q}^L = s^L\left(\mathbf{n}^L\otimes\mathbf{n}^L - \frac{1}{3}\mathbf{I}\right)$ *be a uniaxial small energy solution of (26) in* $\mathcal{A}_{\mathbf{Q}}$, *for* L *sufficiently small. Then for* $\mathbf{x}\in\Omega\setminus B_\delta(S_0)$, *we have*

$$\begin{aligned} &|\nabla s^L| \leq \epsilon_1(\mathbf{x}) \\ &\left||\nabla \mathbf{n}^L(\mathbf{x})|^2 - |\nabla \mathbf{n}_0|^2\right| \leq \epsilon_2(\mathbf{x}) \end{aligned} \tag{106}$$

where $\mathbf{n}_0$ *and* $\mathbf{Q}^0$ *are defined in (12) and* $\epsilon_1, \epsilon_2 \to 0^+$ *as* $L\to 0^+$.

Proof: Lemma 3 is a direct consequence of Proposition 4. Let $\mathbf{x}\in\Omega\setminus B_\delta(S_0)$. Then from Proposition 4, we have that

$$\begin{aligned} &\left|\mathbf{Q}^L_{ij}(\mathbf{x}) - \mathbf{Q}^0_{ij}(\mathbf{x})\right| \leq \epsilon_3(\mathbf{x}) \\ &\left|\mathbf{Q}^L_{ij,k}(\mathbf{x}) - \mathbf{Q}^0_{ij,k}(\mathbf{x})\right| \leq \epsilon_4(\mathbf{x}) \end{aligned} \tag{107}$$

where $\mathbf{Q}^0$ is the limiting harmonic map in (12), $\mathbf{Q}_{ij,k} = \frac{\partial \mathbf{Q}_{ij}}{\mathbf{x}_k}$ and $\epsilon_3, \epsilon_4 << 1$. One can directly compute

$$\left|\nabla \mathbf{Q}^0\right|^2 = 2s_+^2\left|\nabla \mathbf{n}_0\right|^2. \tag{108}$$

On the other hand,

$$\left|\mathbf{Q}^L\right|^2 = \frac{2}{3}(s^L)^2$$

and therefore,

$$\mathbf{Q}^L_{ij}\mathbf{Q}^L_{ij,k} = \frac{2}{3}s^L\partial_k s^L \tag{109}$$

where $|s^L(\mathbf{x}) - s_+| < \epsilon_5(\mathbf{x}) << 1$ for $\mathbf{x} \in \Omega \setminus B_\delta(S_0)$, from (40).

One can re-write $\mathbf{Q}^L_{ij}\mathbf{Q}^L_{ij,k}$ as shown below -

$$\mathbf{Q}^L_{ij}\mathbf{Q}^L_{ij,k} = (\mathbf{Q}^L_{ij}(\mathbf{x}) - \mathbf{Q}^0_{ij}(\mathbf{x}))\mathbf{Q}^L_{ij,k}(\mathbf{x}) + \mathbf{Q}^0_{ij}(\mathbf{x})\left(\mathbf{Q}^L_{ij,k}(\mathbf{x}) - \mathbf{Q}^0_{ij,k}(\mathbf{x})\right) \tag{110}$$

since $\mathbf{Q}^0_{ij}\mathbf{Q}^0_{ij,k} = 0$ from $|\mathbf{Q}^0|^2 = \frac{2}{3}s_+^2$. Using the inequalities (107), the global bound (79) and the triangle inequality, we have that

$$\left|\mathbf{Q}^L_{ij}(\mathbf{x})\mathbf{Q}^L_{ij,k}(\mathbf{x})\right| \leq \epsilon_6(\mathbf{x}) << 1 \tag{111}$$

for $\mathbf{x} \in \Omega \setminus B_\delta(S_0)$ and from (109) and (40), this necessarily implies that

$$|\nabla s^L| \leq \epsilon_7\left(L\right) \tag{112}$$

away from S_0, where $\epsilon_7 \to 0^+$ as $L \to 0^+$.

On the other hand, from Proposition 4, $\mathbf{Q}^L \to \mathbf{Q}^0$ in $C^{1,\alpha}(\Omega; \bar{S}_3)$ as $L \to 0$ (up to a subsequence), everywhere away from S_0. Therefore, for $\mathbf{x} \in \Omega \setminus B_\delta(S_0)$,

$$\left||\nabla\mathbf{Q}^L|^2 - |\nabla\mathbf{Q}^0|^2\right| \leq \epsilon_8(\mathbf{x}) \tag{113}$$

where $\epsilon_8 \to 0^+$ as $L \to 0^+$. A direct computation shows that

$$|\nabla\mathbf{Q}^L|^2 = \frac{2}{3}|\nabla s^L|^2 + 2(s^L)^2|\nabla\mathbf{n}^L|^2.$$

Combining (40), (112), (113) and (108), we have that $|\nabla\mathbf{n}^L|^2 \to |\nabla\mathbf{n}_0|^2$ as $L \to 0^+$. Lemma 3 now follows. $\square$

Proposition 5 *Let* $\mathbf{Q}^L = s^L\left(\mathbf{n}^L \otimes \mathbf{n}^L - \frac{1}{3}\mathbf{I}\right)$ *be a uniaxial small energy solution of (26) in* $\mathcal{A}_\mathbf{Q}$*, for* L *sufficiently small. Then for* $\mathbf{x} \in \Omega \setminus B_\delta(S_0)$*, we have that*

$$\left|\frac{s_+ - s^L}{L} - \frac{9\left|\nabla\mathbf{n}_0\right|^2}{\sqrt{b^4 + 24a^2c^2}}\right| \leq \epsilon_9(\mathbf{x}) \tag{114}$$

where $\epsilon_9 \to 0^+$ *as* $L \to 0^+$.

Proof: Consider the function $\psi^L = \frac{s_+ - s^L}{L}$ in (99) and the equation (47) on $\Omega \setminus B_\delta(S_0)$

$$\Delta s^L - 3s^L|\nabla\mathbf{n}^L|^2 = -2c^2\frac{s^L}{3}(s^L - s_-)\psi^L \tag{115}$$

where $s_\pm = \frac{b^2 \pm \sqrt{b^4 + 24a^2c^2}}{4c^2}$. Equation (115) can be re-arranged to give

$$-L\Delta\left(\psi^L - \frac{9|\nabla\mathbf{n}_0|^2}{\sqrt{b^4 + 24a^2c^2}}\right) + 2c^2\frac{s^L(s^L - s_-)}{3}\left(\psi^L - \frac{9|\nabla\mathbf{n}_0|^2}{\sqrt{b^4 + 24a^2c^2}}\right) =$$

$$= 3s^L|\nabla\mathbf{n}^L|^2 + \frac{9L}{\sqrt{b^4 + 24a^2c^2}}\Delta\left|\nabla\mathbf{n}_0\right|^2 - \frac{6c^2 s^L\left(s^L - s_-\right)}{\sqrt{b^4 + 24a^2c^2}}\left|\nabla\mathbf{n}_0\right|^2. \tag{116}$$

We note that $\Delta\left|\nabla \mathbf{n}_0\right|^2 = O(1)$ away from S_0 and the right-hand side of (116) can be written as

$$3s^L|\nabla\mathbf{n}^L|^2 + \frac{9L}{\sqrt{b^4+24a^2c^2}}\Delta\left|\nabla\mathbf{n}_0\right|^2 - \frac{6c^2 s^L\left(s^L - s_-\right)}{\sqrt{b^4+24a^2c^2}}\left|\nabla\mathbf{n}_0\right|^2 = \tag{117}$$

$$= 3s^L|\nabla\mathbf{n}^L|^2 - 3s_+\left|\nabla\mathbf{n}_0\right|^2 + 3s_+\left|\nabla\mathbf{n}_0\right|^2 - \frac{6c^2 s^L\left(s^L - s_-\right)}{\sqrt{b^4+24a^2c^2}}\left|\nabla\mathbf{n}_0\right|^2 + O(L). \tag{118}$$

Finally, we use (40) and (106) to deduce that

$$3s^L|\nabla\mathbf{n}^L|^2 - 3s_+\left|\nabla\mathbf{n}_0\right|^2 \leq \epsilon_{10}$$

where $\epsilon_{10} \to 0^+$ as $L \to 0^+$ and

$$\frac{6c^2 s^L\left(s^L - s_-\right)}{\sqrt{b^4+24a^2c^2}}\left|\nabla\mathbf{n}_0\right|^2 \to 3s_+\left|\nabla\mathbf{n}_0\right|^2$$

as $L \to 0^+$, since $s^L - s_- \to (s_+ - s_-) = \sqrt{b^4+24a^2c^2}/2c^2$ as $L \to 0^+$. Combining the above, we have that

$$-L\Delta\left(\psi^L - \frac{9|\nabla\mathbf{n}_0|^2}{\sqrt{b^4+24a^2c^2}}\right) + \beta\left(\psi^L - \frac{9|\nabla\mathbf{n}_0|^2}{\sqrt{b^4+24a^2c^2}}\right) \leq \epsilon_{11} \tag{119}$$

where β is a positive constant independent of L and $\epsilon_{11} \to 0^+$ as $L \to 0^+$. Proposition 5 now follows from the maximum principle and Lemma 2 of [4]. □

7 Biaxial case in $3D$: Interior estimates

Consider a biaxial small energy sequence of solutions of (26), $\left\{\mathbf{Q}^{L_k}\right\}$, in the admissible space $\mathcal{A}_{\mathbf{Q}}$ where $L_k \to 0^+$ as $k \to \infty$. From Section 4, $\left\{\mathbf{Q}^{L_k}\right\}$ converges strongly to a limiting harmonic map $\mathbf{Q}^0$ (as in (12)) in $W^{1,2}(\Omega, \bar{S}_3)$ (up to a subsequence) [15], for $L_k \to 0^+$ as $k \to \infty$. Further, we can use the interior and boundary monotonicity lemmas (36) and (37) to show that

$$f_B\left(\mathbf{Q}^{L_k}\right) \to 0 \tag{120}$$

uniformly everywhere away from the singular set, S_0, of the limiting harmonic map or equivalently

$$s \to s_+, \quad r \to 0^+ \tag{121}$$

uniformly away from S_0, as $k \to \infty$ [15].

In what follows, we derive the analogue of Lemma 2 in the biaxial case.

Lemma 4 *Let $\mathbf{Q}^L$ be an arbitrary small energy solution of (26), for L sufficiently small. Let*

$$A^L = \frac{1}{2}\mathbf{Q}^L_{ij,k}\mathbf{Q}^L_{ij,k}.$$

Then on $\Omega \setminus B_\delta(S_0)$, we have the following inequality

$$-\Delta A^L + \left|\nabla^2\mathbf{Q}^L\right|^2 \leq \frac{1}{\alpha^2}\left|\nabla^2\mathbf{Q}^L\right|^2 + \alpha^4\frac{{A^L}^2}{|\mathbf{Q}^L|^2} \tag{122}$$

where $B_\delta(S_0)$ is a small δ-neighbourhood of S_0 and $\alpha > 1$ is a positive constant independent of L.

Proof: We start with the relation (74)

$$\Delta A^L = |\nabla^2 \mathbf{Q}^L|^2 + \mathbf{Q}^L_{ij,k}\mathbf{Q}^L_{ij,ppk}$$

and drop the superscript L for brevity.

We need to estimate $|\mathbf{Q}_{ij,k}\mathbf{Q}_{ij,ppk}|$ in terms of $|\Delta\mathbf{Q}|\,|\nabla\mathbf{Q}|^2/|\mathbf{Q}|$. Straightforward but tedious calculations show that

$$\begin{aligned}
&L^2\,|\mathbf{Q}_{ij,k}\mathbf{Q}_{ij,ppk}|^2 = a^4|\nabla\mathbf{Q}|^4 + c^4\left(\mathrm{tr}\mathbf{Q}^2\right)^2|\nabla\mathbf{Q}|^4 + 4b^4\left(\mathbf{Q}_{ip}\mathbf{Q}_{pj,q}\mathbf{Q}_{ij,q}\right)^2 + \\
&+4a^2b^2\mathbf{Q}_{ip}\mathbf{Q}_{pj,q}\mathbf{Q}_{ij,q}|\nabla\mathbf{Q}|^2 - 4b^2c^2|\mathbf{Q}|^2|\nabla\mathbf{Q}|^2\mathbf{Q}_{ip}\mathbf{Q}_{pj,q}\mathbf{Q}_{ij,q} - 2a^2c^2|\mathbf{Q}|^2|\nabla\mathbf{Q}|^4 + \\
&+4c^4\left(\mathbf{Q}\cdot\nabla\mathbf{Q}\right)^4 + 4c^4\left(\mathbf{Q}\cdot\nabla\mathbf{Q}\right)^2|\mathbf{Q}|^2|\nabla\mathbf{Q}|^2 - 4a^2c^2|\nabla\mathbf{Q}|^2\left(\mathbf{Q}\cdot\nabla\mathbf{Q}\right)^2 - 8b^2c^2\left(\mathbf{Q}\cdot\nabla\mathbf{Q}\right)^2\mathbf{Q}_{ip}\mathbf{Q}_{pj,q}\mathbf{Q}_{ij,q} \leq \\
&\leq C(a^2,b^2,c^2)|\nabla\mathbf{Q}|^4
\end{aligned} \tag{123}$$

where we have used the Euler-Lagrange equations (26) to compute the right-hand side of (123) and the uniform convergence of the bulk energy density to its minimum value away from the singular set of the limiting harmonic map. It can be shown that the right-hand side of (123) vanishes for $\mathbf{Q}\in\mathbf{Q}_{\min}$, where $\mathbf{Q}_{\min}$ has been defined in (7). The details of these calculations are omitted here for brevity.

Secondly,

$$\begin{aligned}
&L^2\frac{|\nabla\mathbf{Q}|^4}{|\mathbf{Q}|^2}|\Delta\mathbf{Q}|^2 = a^4|\nabla\mathbf{Q}|^4 + 2a^2b^2|\nabla\mathbf{Q}|^4\frac{\mathrm{tr}\mathbf{Q}^3}{|\mathbf{Q}|^2} - 2a^2c^2|\mathbf{Q}|^2|\nabla\mathbf{Q}|^4 \\
&-2b^2c^2\mathrm{tr}\mathbf{Q}^3|\nabla\mathbf{Q}|^4 + c^4|\mathbf{Q}|^4|\nabla\mathbf{Q}|^4 + 2b^4\frac{s^4+r^4+3s^2r^2-2s^3r-2sr^3}{27|\mathbf{Q}|^2}|\nabla\mathbf{Q}|^4 \geq D(a^2,b^2,c^2)|\nabla\mathbf{Q}|^4
\end{aligned} \tag{124}$$

where

$$D(a^2,b^2,c^2) = 0$$

if and only if $\mathbf{Q}\in\mathbf{Q}_{\min}$.

Combining (123) and (124), we get that

$$|\mathbf{Q}_{ij,k}\mathbf{Q}_{ij,ppk}| \leq D^{'}(a^2,b^2,c^2)\frac{|\nabla\mathbf{Q}|^2}{|\mathbf{Q}|}|\Delta\mathbf{Q}| \tag{125}$$

where $D^{'}$ is a positive constant independent of L. Substituting (125) into (74) and repeating the same steps as in Lemma 2, (122) follows. The proof of Lemma 4 is then complete. $\square$

Corollary: Let $\mathbf{Q}^L$ be a biaxial small energy solution of (26) in the admissible space $\mathcal{A}_{\mathbf{Q}}$, for L sufficiently small. Then we have the following interior estimates, away from the singular set, S_0, of the limiting harmonic map $\mathbf{Q}^0$ in (12) :-

$$\frac{1}{2}|\nabla\mathbf{Q}^L|^2 + \frac{f_B(\mathbf{Q}^L)}{L} \leq H(a^2,b^2,c^2,\Omega) \tag{126}$$

$$|\mathbf{Q}^0| - |\mathbf{Q}^L| \leq C(a^2,b^2,c^2)L \quad \text{on } K\subset\Omega\setminus B_\delta(S_0). \tag{127}$$

In particular, the largest positive eigenvalue, λ_1^L, of $\mathbf{Q}^L$, satisfies the following inequality on the interior compact subset $K\subset\Omega\setminus B_\delta(S_0)$

$$\frac{2s_+}{3} - \lambda_1^L \leq D(a^2,b^2,c^2)L \tag{128}$$

where s_+ has been defined in (8) and the positive constants H,C and D are independent of L.

Proof: The inequality (126) is a mere repetition of (43); see [15] for a proof.

Consider the function

$$\left|\mathbf{Q}^L\right| = \left(\mathbf{Q}^L_{pq}\mathbf{Q}^L_{pq}\right)^{1/2} \quad p,q=1,2,3.$$

Then a direct computation shows that $|\mathbf{Q}^L|$ satisfies the following partial differential equation

$$\Delta|\mathbf{Q}| = \frac{|\nabla\mathbf{Q}|^2}{|\mathbf{Q}|} - \frac{(\mathbf{Q}\cdot\nabla\mathbf{Q})^2}{|\mathbf{Q}|^3} + \frac{\mathbf{Q}_{rs}\Delta\mathbf{Q}_{rs}}{|\mathbf{Q}|} \quad r,s=1\dots 3 \tag{129}$$

where $(\mathbf{Q}\cdot\nabla\mathbf{Q})^2 = \frac{1}{4}\left|\nabla|\mathbf{Q}|^2\right|^2$ and we have dropped the superscript L for brevity.

On the interior compact subset $K\subset\Omega\setminus B_\delta(S_0)$, we have the following inequalities

$$\begin{aligned}&\frac{2}{3}s_+^2 - \epsilon_1 \leq |\mathbf{Q}|^2 \leq \frac{2}{3}s_+^2\\ &|\nabla\mathbf{Q}|^2 \leq C_1(a^2,b^2,c^2)\end{aligned} \tag{130}$$

where we have used (31), (120) and (126). Therefore, the first two terms on the right-hand side of (129) can be bounded independently of L. We use the Euler-Lagrange equations (26) to compute the third term on the right-hand side of (129) i.e.

$$\frac{\mathbf{Q}_{rs}\Delta\mathbf{Q}_{rs}}{|\mathbf{Q}|} = \frac{1}{|\mathbf{Q}|L}\left\{-a^2|\mathbf{Q}|^2 - b^2\mathrm{tr}\mathbf{Q}^3 + c^2|\mathbf{Q}|^4\right\} = \frac{|\mathbf{Q}|}{L}\left\{c^2|\mathbf{Q}|^2 - \frac{b^2|\mathbf{Q}|}{\sqrt{6}} - a^2\right\} + \frac{b^2|\mathbf{Q}|^2}{\sqrt{6}L}\left(1-\sqrt{6}\frac{\mathrm{tr}\mathbf{Q}^3}{|\mathbf{Q}|^3}\right).$$

We recall from [15] that

$$\beta^2(\mathbf{Q}) = 1 - 6\left(\frac{\mathrm{tr}\mathbf{Q}^3}{|\mathbf{Q}|^3}\right)^2 \in [0,1]$$

is the biaxiality parameter and as a direct consequence of (126), we have

$$\beta^2(\mathbf{Q}) = 1 - 6\left(\frac{\mathrm{tr}\mathbf{Q}^3}{|\mathbf{Q}|^3}\right)^2 \leq C_2(a^2,b^2,c^2)L$$

on the compact interior subset $K\subset\Omega\setminus B_\delta(S_0)$, for a positive constant C_2 independent of L. Further, we have the following sequence of inequalities on $K\subset\Omega\setminus B_\delta(S_0)$

$$C_3(a^2,b^2,c^2)\left(|\mathbf{Q}| - |\mathbf{Q}^0|\right) \leq \left\{c^2|\mathbf{Q}|^2 - \frac{b^2|\mathbf{Q}|^2}{\sqrt{6}} - a^2\right\} \leq C_4(a^2,b^2,c^2)\left(|\mathbf{Q}| - |\mathbf{Q}^0|\right)$$

for positive constants C_3, C_4 independent of L (see (120) and (70)).

From the preceding remarks, we deduce that

$$\Delta|\mathbf{Q}|(\mathbf{x}) \leq \alpha(a^2,b^2,c^2) + C_4(a^2,b^2,c^2)\frac{\left(|\mathbf{Q}|(\mathbf{x}) - |\mathbf{Q}^0|(\mathbf{x})\right)}{L}, \quad \mathbf{x}\in\Omega\setminus B_\delta(S_0) \tag{131}$$

where α is a positive constant independent of L. Define the function

$$\psi = \frac{\left(|\mathbf{Q}^0| - |\mathbf{Q}|\right)}{L}.$$

Then using (131), we see that ψ satisfies the following inequality on $K \subset \Omega \setminus B_\delta(S_0)$

$$-L\Delta\psi + \beta(a^2, b^2, c^2)\psi \leq \alpha^{'}(a^2, b^2, c^2). \tag{132}$$

Finally, we apply the maximum principle and Lemma 2 in [4] to deduce that

$$|\psi(\mathbf{x})| \leq \gamma(a^2, b^2, c^2) \quad \mathbf{x} \in \Omega \setminus B_\delta(S_0), \tag{133}$$

for positive constants $\alpha^{'}, \beta$ and γ independent of L and (127) follows. The inequality (127) improves upon a previous estimate in [15] where an analysis of the bulk energy density f_B, coupled with (120) and (126), shows that $|\mathbf{Q}^0| - |\mathbf{Q}| \leq A(a^2, b^2, c^2)\sqrt{L}$, for a positive constant $A(a^2, b^2, c^2)$ independent of L.

For (128), we use the following alternative representation formula to (1)

$$\mathbf{Q}^L = S_L \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\right) + R_L \left(\mathbf{m} \otimes \mathbf{m} - \mathbf{p} \otimes \mathbf{p}\right) \tag{134}$$

where $\mathbf{n}, \mathbf{m}$ and $\mathbf{p}$ are the orthonormal eigenvectors and

$$0 \leq s_+ - S_L \leq C_6\sqrt{L}; \quad R_L^2 \leq C_5 L \tag{135}$$

on the interior compact subset $K \subset \Omega \setminus B_\delta(S_0)$, for positive constants C_6, C_5 independent of L (see (120) and Proposition 7 in [15]). We note that

$$|\mathbf{Q}|^2 = \frac{2}{3}S_L^2 + 2R_L^2$$

and hence the inequality (127) necessarily implies that

$$s_+ - S_L\left(1 + \frac{3R_L^2}{S_L^2}\right)^{1/2} \leq C_7 L,$$

for a positive constant C_7 independent of L. This combined with (135) i.e. $R_L^2 \leq C_5 L$ yields the improved estimate

$$0 \leq s_+ - S_L(\mathbf{x}) \leq C_8 L \quad \mathbf{x} \in \Omega \setminus B_\delta(S_0) \tag{136}$$

where $C_8 > 0$ is independent of L. Finally, it suffices to note from (134) that the largest positive eigenvalue of $\mathbf{Q}^L$ is given by

$$\lambda_1^L = \frac{2}{3}S_L$$

and (128) directly follows from (136). $\Box$

Let $\mathbf{Q}^L = S_L\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\right) + R_L\left(\mathbf{m} \otimes \mathbf{m} - \mathbf{p} \otimes \mathbf{p}\right)$ be an arbitrary Landau-de Gennes minimizer in the admissible space $\mathcal{A}_{\mathbf{Q}}$, for L sufficiently small. In [15], we establish that an arbitrary Landau-de Gennes minimizer is either purely uniaxial everywhere or is biaxial everywhere except for possibly a set, Ψ_L, of zero Lebesgue measure interfaces. Then the eigenvectors $\mathbf{n}$ and $\mathbf{m}$ are analytic everywhere away from $S_0 \cup \Psi_L$ [27] and S_L and R_L are constrained by the inequalities (136), everywhere away from S_0. The following equations hold on an interior compact set $K \subset \Omega$, that does not contain any singularities of $\mathbf{Q}^0$ and does not intersect Ψ_L.

Corollary: Let $\mathbf{Q}^L$ be an arbitrary Landau-de Gennes global minimizer in the admissible space $\mathcal{A}_{\mathbf{Q}}$, for L sufficiently small. Let $K \subset \Omega \setminus \{B_\delta(S_0) \cup B_\sigma(\Psi_L)\}$ where δ and σ are positive constants independent of L. Then the following equations hold everywhere on K:

$$\Delta S_L - 3S_L|\nabla \mathbf{n}|^2 + 3R_L\left[(\mathbf{n}\cdot\nabla\mathbf{m})^2 - (\mathbf{n}\cdot\nabla\mathbf{p})^2\right] = \frac{1}{3L}\left(2c^2S_L^3 - b^2S_L^2 - 3a^2S_L + 6c^2S_LR_L^2 + 3b^2R_L^2\right) \tag{137}$$

$$\Delta R_L - R_L\left(|\nabla\mathbf{m}|^2 + |\nabla\mathbf{p}|^2\right) + \left[S_L(\mathbf{m}\cdot\nabla\mathbf{n})^2 - S_L(\mathbf{p}\cdot\nabla\mathbf{n})^2 - 2R_L(\mathbf{m}\cdot\nabla\mathbf{p})^2\right] = $$
$$= \frac{1}{L}\left(2c^2R_L^3 + \frac{2c^2S_L^2R_L}{3} + \frac{2b^2S_LR_L}{3} - a^2R_L\right). \tag{138}$$

It follows from (137) and (138) that

$$|R_L|(\mathbf{x}) \leq Q(a^2,b^2,c^2)L \quad \mathbf{x}\in K \subset \Omega\setminus\{B_\delta(S_0)\cup B_\sigma(\Psi_L)\} \tag{139}$$

where Q is a positive constant independent of L.

Proof: We drop the superscript L from $\mathbf{Q}^L$ and the subscript L from S_L, R_L for convenience. The equations (137) and (138) follow from tedious but straightforward manipulations of the Euler-Lagrange equations (26). To see (139), we note that $R^2 \leq Q^{'}L$ and $0 \leq s_+ - S_L \leq Q^*L$ (from (135) and (136)) and $|\nabla\mathbf{Q}|^2 \leq Q^{**}L$ (from (126)) on the interior compact subset K, where $Q^{'}, Q^*, Q^{**}$ are positive constants independent of L. Therefore, all terms on the left-hand side of (138) can be bounded independently of L in the limit $L \to 0^+$. On the other hand, the terms on the right-hand side of (138) can be bounded independently of L, in the limit $L\to 0^+$, if and only if $|R| \leq Q^{''}L$, for a positive constant $Q^{''}$ independent of L. The inequality (139) now follows. □

8 Generalizations

This paper focuses on qualitative properties of small energy sequences of solutions associated with the Landau-de Gennes energy functional on $2D$ and $3D$ domains. This is a general framework that includes local and global energy minimizers. In the $2D$ case, we focus on energy minimizers, show that the Landau-de Gennes theory is equivalent to Ginzburg-Landau theory for superconductors and make predictions about the dimension of the defect set, the defect locations and the asymptotic profile of global minimizers close to and far away from the defect set.

In $3D$, we focus on the vanishing core limit, expressed in terms of a dimensionless parameter $L \to 0$, which is relevant for macroscopic domains that are much larger than the uniaxial correlation length. We emphasize on uniaxial small energy sequences because this is the first step in a rigorous study of arbitrary minimizers. The topological defects are contained inside the corresponding isotropic sets. We derive the governing equations for the scalar order parameter s^L and the leading eigenvector $\mathbf{n}^L$; these equations reflect the coupling between the two quantities. We show that the topological defects (or equivalently the isotropic set) are necessarily contained in a small neighbourhood of the singular set of a limiting harmonic map and establish the vortex-like or radial hedgehog-like profile of isolated point defects. We also study the qualitative properties of uniaxial small energy solutions away from the isotropic set. In particular, we establish the $C^{1,\alpha}$-convergence of uniaxial small energy sequences to a limiting harmonic map, everywhere away from the isotropic set, in the vanishing core limit. We use this convergence result to obtain an expansion for the scalar order parameter s^L in terms of L, everywhere away from the isotropic set. As mentioned in Section 2, a limiting harmonic map is an energy minimizer within the Oseen-Frank theory for uniaxial liquid crystals with constant order parameter. These convergence results suggest that Oseen-Frank theory and Landau-de Gennes theory give qualitatively similar information away from topological defects and the Landau-de Gennes theory can potentially give new information near topological defects.

Such uniaxial small energy sequences do exist, such as *radial-hedgehog solutions* [17]. Let Ω be the unit ball centered at the origin, in three dimensions with radial anchoring conditions: $\mathbf{Q}_b = s_+\left(\frac{\mathbf{r}}{|\mathbf{r}|} \otimes \frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{I}\right)$. Then the limiting harmonic map $\mathbf{Q}^0$ is unique [13] and is given by

$$\mathbf{Q}^0 = s_+\left(\frac{\mathbf{r}}{|\mathbf{r}|} \otimes \frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{I}\right).$$

We can explicitly construct a family of radial-hedgehog type solutions of (26) for each $L > 0$ [17]

$$\mathbf{Q}_L = s_L(|\mathbf{r}|)\left(\frac{\mathbf{r}}{|\mathbf{r}|} \otimes \frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{I}\right)$$

such that

$$\mathcal{I}_{\mathcal{LG}}[\mathbf{Q}_L] \leq \mathcal{I}_{\mathcal{LG}}[\mathbf{Q}^0] = 8\pi s_+^2$$

for all $L > 0$. This radial hedgehog sequence $\{\mathbf{Q}_L\}$ is an example of a uniaxial small energy sequence. We note that $\mathbf{Q}_L$ has a single isolated zero at the origin, has a hedgehog-type profile around the origin (as predicted by Proposition 2) and the results in Section 6 apply everywhere away from the origin. Further, $\mathbf{Q}_L$ has complete radial symmetry and any symmetry-breaking is likely to have an energy-penalty. This makes $\mathbf{Q}_L$ a natural candidate for a uniaxial minimizer in the admissible class $\mathcal{A}_{\mathbf{Q}}$, in the case of Ω being a unit ball. We will investigate this in future work.

Our results in the biaxial case are restricted to interior estimates, away from the singular set of a limiting harmonic map. At present, we cannot obtain uniform bounds for the gradient of a small energy solution up to the boundary. We obtain physically relevant interior estimates away from singularities, in the vanishing core limit and these include estimates for the solution norm and the eigenvalues of the small energy solutions. We also derive the governing equations for the scalar order parameters and these equations will be useful for an asymptotic study of arbitrary biaxial solutions.

A complete analysis of Landau-de Gennes global energy minimizers can be accomplished only if we have a better understanding of the full Euler-Lagrange equations (26). One strategy is to decompose the system (26) as follows -

$$\begin{aligned} L\Delta\mathbf{Q}_{ij} &= -a^2\mathbf{Q}_{ij} - b^2\left(\mathbf{Q}_{ik}\mathbf{Q}_{kj} - \frac{\delta_{ij}}{3}\mathrm{tr}(\mathbf{Q}^2)\right) + c^2\mathbf{Q}_{ij}\mathrm{tr}(\mathbf{Q}^2) = \\ &= \left(-a^2 - b^2\frac{|\mathbf{Q}|}{\sqrt{6}} + c^2|\mathbf{Q}|^2\right)\mathbf{Q}_{ij} + b^2\left(\frac{|\mathbf{Q}|}{\sqrt{6}}\mathbf{Q}_{ij} - \mathbf{Q}_{ik}\mathbf{Q}_{kj} + \frac{1}{3}|\mathbf{Q}|^2\delta_{ij}\right) \end{aligned} \tag{140}$$

where we can think of the first term as being a *Ginzburg-Landau* component (because of its similarity to Ginzburg-Landau equations for superconductors [18]) and the second term as being a *remainder* component. We need to understand the coupling between the *Ginzburg-Landau* and the *remainder* components and to establish quantitative estimates on the magnitude of the remainder component, in order to derive rigorous results for the structure of global Landau-de Gennes energy minimizers and their relation to the limiting harmonic map $\mathbf{Q}^0$ in (12). Other future directions are to characterize defects in global minimizers (uniaxial versus biaxial cases), to study qualitative properties of minimizers for different choices of the boundary conditions i.e. when $\mathbf{Q}_b \notin \mathbf{Q}_{\min}$ where $\mathbf{Q}_{\min}$ has been defined in (7) and to study minimizers in different temperature regimes. We plan to report on these problems in future work.

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